Inelastic carrier lifetime in a coupled graphene electron-phonon system: Role of plasmon-phonon coupling

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We calculate the inelastic scattering rates and the hot electron inelastic mean free paths for both monolayer and bilayer graphene on a polar substrate. We study the quasiparticle self-energy by taking into account both electron-electron and electron-surface optical (SO) phonon interactions. In this calculation the leading order dynamic screening approximation (G0W approximation) is used to obtain the quasiparticle self-energy by treating electrons and phonons on an equal footing. We find that the strong coupling between the SO phonon and plasmon leads to a new decay channel for the quasiparticle through the emission of the coupled mode, and gives rise to an abrupt increase in the scattering rate, which is absent in the uncoupled system. In monolayer graphene a single jump in the scattering rate occurs, arising from the emission of the low energy branch of the coupled plasmon-phonon modes. In bilayer graphene the emission of both low and high energy branches of the coupled modes contributes to the scattering rate and gives rise to two abrupt changes in the scattering rate. The jumps in the scattering rate can be potentially used in the hot electron device such as switching devices and oscillators.

I. INTRODUCTION

Two dimensional (2D) graphene has been extensively studied during recent years because of its fundamental and technological interest. In most of currently available graphene samples (i.e., graphene field effect transistors) graphene lies on top of a polar substrate such as SiO$_2$, SiC, or HfO. In such graphene samples the polar optical phonons of the substrate are localized near the graphene-substrate interface, and free carriers in graphene couple to the surface polar (SO) phonons of the underlying substrate through the long-range polar Fröhlich coupling. In polar materials the longitudinal optical (LO) phonons generate a long-range electric field which scatters electrons, and typically their contribution to resistivity is dominant at room temperatures. In non-polar materials such as graphene, however, the non-polar optical phonons have little effect on carrier transport because the long-range interaction between electrons and phonons is absent and the energy of the (non-polar) optical phonon is very high, $\sim 200$ meV. For this reason, the SO phonons rather than non-polar LO or acoustic phonons can be the dominant scattering source at room temperature in graphene on a polar substrate.

In addition to being the main scattering source in transport, it is well known that in polar materials the electron-polar optical phonon interaction leads to polaronic many-body renormalization of the single particle properties, e.g., polaronic Fermi velocity (effective mass) renormalization and broadening of the quasiparticle spectral function. Even though these effects are expected to be small in graphene due to the weak Fröhlich coupling arising from the spatial separation between electrons in graphene and the surface of a substrate and due to the large dielectric constant of the substrate, there is a much stronger quantitative manifestation of electron-SO phonon coupling in graphene on a polar substrate, which is the macroscopic coupling of the electronic collective modes (i.e., plasmons) to the SO phonons of the system via the long-range Fröhlich coupling. This mode coupling phenomena, which hybridizes the collective plasmon modes of the electron gas with the SO-phonon modes of the substrate, gives rise to the coupled plasmon-phonon modes, which have been extensively studied both experimentally and theoretically in graphene. The plasmon-phonon coupling is important in many single particle properties including the inelastic carrier life time, hot-electron energy-loss processes, and transport properties.

The objective of this paper is to provide the inelastic carrier lifetime and the inelastic mean free path of monolayer and bilayer graphene in the presence of the long-range polar Fröhlich coupling between electrons in graphene and SO phonons in the underlying polar substrate within the leading order perturbation theory, i.e., G$_0$W approximation. We consider the effective total interaction (i.e., the coupled electron-electron and electron-SO phonon interaction) within the framework of the random phase approximation (RPA). Even though the problem is treated within the G$_0$W framework of the leading order effective interaction approximation, our results should be quite valid in graphene because graphene has a very weak Fröhlich coupling, which justifies the neglect of the electron-phonon vertex corrections. We include, however, important physical effects of the dynamical screening, phonon self-energy correction, plasmon-phonon mode coupling, and Landau damping. In the presence of electron-SO phonon coupling we find new features in the inelastic carrier life time, which is obviously absent without the coupling.
There have been several studies upon the effects of electron-SO phonon interaction in graphene.\textsuperscript{15–17} Various many-body quantities such as self-energy, scattering rate and spectral function have been calculated for the statically screened electron-SO phonon interaction. Such calculations based on the static screening approximation are justified when the charge carrier density is high enough that the corresponding Fermi energy exceeds the SO phonon energy. However, the SO phonon energies of the common polar substrates for graphene such as SiC or SiO$_2$ range from 50 meV to 200 meV, and they are comparable to the typical Fermi energies of graphene, 100 – 300 meV. Thus the dynamic screening of the electron-SO phonon interaction is more desirable. In addition, because the SO phonon energy and the energy of electrons are comparable, we cannot treat the electron-electron interaction and the electron-SO phonon interaction separately. Therefore, we need to treat both interactions equivalently within the same dynamic screening approximation. Quasiparticle properties of various systems have been calculated considering both electron-electron and electron-phonon interactions.\textsuperscript{18,19} However, there has been no calculation of quasiparticle properties of graphene on a polar substrate with both electron-electron and electron-SO phonon interactions being equally treated.

In this paper, we calculate the scattering rate ($\tau^{-1}$) and the corresponding inelastic mean free path ($l$) of quasiparticles in both monolayer and bilayer graphene by taking into account both electron-electron and electron-SO phonon interactions. We also investigate the effect of the dynamic screening of the electron-SO phonon interaction and plasmon-phonon coupling. In addition, we propose a possible technological application to a lateral hot electron transistor by making use of the electron-SO phonon interaction effect. Throughout the paper, we refer to the graphene system with both electron-electron and electron-SO phonon interactions as the coupled system, whereas the graphene system only with the electron-electron interaction as the uncoupled system.

The paper is organized as follows. In Section II the generalized theory is presented to calculate the electron self-energy in the presence of both electron-electron and electron-SO phonon interactions. Section III presents the results of the scattering rate and the hot electron mean free paths for both monolayer and bilayer graphene. We summarize in Sec. IV with a discussion.

\section{II. THEORY}

In the coupled system, electrons interact with each other through the direct Coulomb interaction $v_{c}(q) = 2\pi e^{2}/\epsilon_{\infty}q$ [Fig. 1(a)] and the SO-phonon mediated interaction $v_{ph}(q, \omega) = M_{0}(q)D_{0}(\omega)$ [Fig. 1(b)]. Here the electron-SO phonon coupling $M_{0}(q)$ is given by

$$M_{0}^{2}(q) = v_{c}(q)\alpha e^{-2qd\omega_{SO}}/2,$$

\hfill (1)

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{(a) Electron-electron Coulomb interaction. (b) Phonon mediated electron-electron interaction. (c) Series of diagrams corresponding to the RPA for the effective interaction in the presence of both electron-electron and electron-phonon interactions. The wiggled (dashed) line represents the electron-electron Coulomb (SO phonon mediated) interaction and $\Pi_{0}$ the bare polarizability.}
\end{figure}

where $d$ is the distance between graphene and the polar substrate.

$$\alpha = \epsilon_{\infty} \left[ \frac{1}{\epsilon_{\infty} + 1} - \frac{1}{\epsilon_{0} + 1} \right],$$

\hfill (2)

$\epsilon_{0}(\epsilon_{\infty})$ is the zero (high) frequency dielectric constant and $D_{0}(\omega)$ is the bare SO-phonon propagator given by

$$D_{0}(\omega) = \frac{2\omega_{SO}}{\omega^{2} - \omega_{SO}^{2}}.$$  \hfill (3)

Within the RPA the effective electron-electron interaction is obtained by the sum of all bare bubble diagrams [Fig. 1(c)] and given by

$$v_{eff}(q, \omega) = \frac{v_{c}(q) + v_{ph}(q, \omega)}{1 - [v_{c}(q) + v_{ph}(q, \omega)]\Pi_{0}(q, \omega)} = \frac{v_{c}(q)}{\epsilon_{1}(q, \omega)},$$

\hfill (4)

where $\Pi_{0}(q, \omega)$ is the bare polarizability of graphene. Thus the total dielectric function from electrons and SO phonons is given by\textsuperscript{11}

$$\epsilon_{1}(q, \omega) = 1 - \frac{2\pi e^{2}}{\epsilon_{\infty}q}\Pi_{0}(q, \omega) + \frac{\alpha e^{-2qd}}{1 - \alpha e^{-2qd} - \omega^{2}/\omega_{SO}^{2}}.$$

\hfill (5)

Here for simplicity we use the zero-temperature polarization as an approximation, which is valid in monolayer graphene at typical doping densities $n = 10^{11} \sim 10^{13}$ cm$^{-2}$ because the corresponding Fermi temperature $T_F = 400 \sim 4000$ K is much larger than room temperature. On the other hand, in bilayer graphene the Fermi temperature at low densities $n \sim 10^{11}$ cm$^{-2}$($T_F \sim 40$ K) is smaller than room temperature, thus the zero temperature approximation is valid only at relatively high densities $n > 10^{12}$ cm$^{-2}$($T_F \sim 400$ K) in bilayer graphene.

Alternatively, the effective interaction $v_{eff}(q, \omega)$ can be written as the sum of the screened electron-electron Coulomb interaction and the screened electron-SO phonon interaction\textsuperscript{6,15}

$$v_{eff}(q, \omega) = \frac{v_{c}(q)}{\epsilon(q, \omega)} + v_{ph}^{sc}(q, \omega),$$

\hfill (6)
where \(\epsilon(q, \omega) = 1 - v_c(q)\Pi_0(q, \omega)\) is the electronic dielectric function within the RPA. The screened electron-SO phonon interaction is given by \(v_{pq}^{\text{sc}}(q, \omega) = [M(q, \omega)]^2 D(q, \omega)\) where \(M(q, \omega) = M_0(q)/\epsilon(q, \omega)\) is the screened interaction matrix element and \(D(q, \omega)\) is the renormalized phonon propagator given by

\[
D(q, \omega) = \frac{D_0(\omega)}{1 - [M_0(\omega)]^2 D_0(\omega)\Pi_0(q, \omega)/\epsilon(q, \omega)}. \tag{7}
\]

Note that the interaction between electrons and SO-phonons is dynamically screened. The effect of dynamic screening in contrast to that of the static screening will be discussed later.

The self-energy of the coupled system within the G\(_0\)W approximation is given by\(^{20}\)

\[
\text{Im}[\Sigma_s(k, \omega)] = \sum_{s'} \int \frac{d^2 q}{(2\pi)^2} [\Theta(\omega - \xi_{k+q,s'}) - \Theta(-\xi_{k+q,s'})] \times \text{Im}[v_{\text{eff}}(q, \omega)] F_{ss'}(k, k + q). \tag{8}
\]

Here, \(s, s' = \pm 1\) are band indices and \(F_{ss'}(k, k + q) = \frac{1}{2} (1 \pm ss' \cos J\theta_{k,k+q})\) is the wavefunction overlap factor with \(J = 1\) \((J = 2)\) for monolayer (bilayer) graphene where \(\theta_{k,k+q}\) is the angle between \(k\) and \(k + q\). Within the on-shell approximation, \(\omega\) is substituted by the on-shell energy \(\xi_{k,s} = \varepsilon_{k,s} - \mu\) where \(\varepsilon_{k,s}\) is the energy dispersion and \(\mu\) is the chemical potential. The scattering rate is given by the imaginary part of the self-energy via the relation \(\hbar/\tau = -2\text{Im}[\Sigma_s^\dagger]\).

### III. RESULTS

#### A. Scattering rate

For numerical calculations, the parameters\(^{20}\) corresponding to SiC are used throughout this paper: \(\hbar\omega_{\text{SO}} = 116.7\ \text{meV}\), \(\varepsilon_{\infty} = 6.4\), \(\epsilon_0 = 10.0\), and \(d = 5\ \text{Å}\). Figures\(^2\)(a) and (b) show the scattering rates for uncoupled and coupled monolayer graphene as a function of the on-shell energy \(\xi_k\). As in the case of the 2D electron gas with the parabolic energy dispersion, the scattering rate vanishes at the Fermi energy (i.e., \(\xi_k = 0\)) and shows the well-known quadratic behavior of \(\sim |\xi_k|^2\ln|\xi_k|\) near the Fermi energy. Away from the Fermi energy, an upward kink structure appears in the scattering rate for the coupled system, whereas the uncoupled system shows no such structure at any energy. Figures\(^2\)(c) and (d) show the calculated loss function of the uncoupled and coupled monolayer graphene for carrier density \(n = 10^{12}\ \text{cm}^{-2}\) with the single-particle excitation (SPE) and the injected-electron energy loss (IEEL) continua. The intersections of the IEEL continua with the SPE continua indicate the allowed quasiparticle decay via the emission of plasmons. Note that the volume of the IEEL continua depends on the energy with which an electron is injected. Hence, an injected electron with a higher energy can have more routes to decay than that injected with a low energy.

For the uncoupled monolayer graphene, the plasmon mode lies outside the SPE\(^{\text{intra}}\) and the quasiparticle cannot decay via plasmon emission because the plasmon dispersion does not enter the IEEL continua over the whole energy range, as shown in Fig.\(^2\)(c). Thus the scattering rate in doped graphene does not show an abrupt increase at any energy.\(^{20}\) On the other hand, as shown in Fig.\(^2\)(d), for the coupled system there are two modes: the phonon-like mode \(\omega_+\) and the plasmon-like mode \(\omega_-\). The plasmon-like mode \(\omega_-\) enters the IEEL continua at a finite critical wave vector \(q_\ell \approx \omega_\text{SO}/(1 - \alpha)/\sqrt{2}\). Thus a new decay channel via \(\omega_-\) emission is turned on around the SO phonon energy \(E_{\text{SO}} = \hbar\omega_{\text{SO}}\), leading to an upward step in the scattering rate. Note that decay via the emission of the phonon-like mode \(\omega_+\) is impossible for monolayer graphene because \(\omega_+\) mode increases linearly at large \(q\) with its energy slightly higher than that of the uncoupled plasmon mode thus it does not enter the IEEL continua.
FIG. 3: Calculated scattering rate as a function of $\xi_k$ for different carrier densities $n = 1, 2, 5, 10 \times 10^{11} \text{ cm}^{-2}$ for (a) uncoupled and (b) coupled bilayer graphene ($J = 2$), and calculated energy loss function for (c) uncoupled and (d) coupled bilayer graphene at $n = 10^{12} \text{ cm}^{-2}$. In (d), the IEEL continua are drawn for two different energies of an injected electron: $\xi_k = 66 \text{ meV}$ (blue dashed line) and $\xi_k = 106.7 \text{ meV}$ (green dashed line). At these energies, the scattering rate increases sharply because the decay via plasmon emission is additionally turned on, as shown in (b).

Figure 3 shows the scattering rate and the loss function in the uncoupled and coupled bilayer graphene. Unlike monolayer graphene, the plasmon dispersions for both uncoupled and coupled bilayer graphene enter the IEEL continua. Therefore, even in the uncoupled system the scattering rate exhibits an abrupt increase, which is absent in the uncoupled monolayer system. In addition, while the coupled monolayer graphene system has only a single jump in the scattering rate, the coupled bilayer graphene shows two abrupt jumps. One of them occurs near $\xi_k \approx E_{SO}$, for which the emission of the phonon-like mode $\omega_-$ damped in the interband SPE is responsible. The other jump occurs due to the emission of the plasmon-like mode $\omega_-$ and its threshold energy strongly depends upon the carrier density, hence the emission of the plasmon-like mode $\omega_-$ is tunable with a carrier density. At higher carrier densities ($E_F > E_{SO}$) the plasmon is strongly coupled to the SO phonon and the threshold energy for the phonon-like mode $\omega_+$ becomes a tunable quantity while the threshold energy for the plasmon-like $\omega_-$ is fixed around the SO phonon energy $E_{SO}$. Note that in bilayer graphene the step of the scattering rate at the phonon-like mode shows a weaker density dependence on the carrier density than that in monolayer graphene because of the constant density of states. Also note that our calculation for bilayer graphene is based on the two band model which is valid only at low carrier densities. At high enough carrier densities, the interlayer coupling becomes negligible and the energy band structure of bilayer graphene behaves as a collection of monolayer graphene sheets, thus we expect that the results for bilayer graphene are similar with those of monolayer graphene.

B. Mean free path

The inelastic mean free paths $l_k = v_k \tau_k$ of the uncoupled and coupled monolayer graphene systems are given in Fig. 4(a). Unlike the uncoupled system, the coupled system shows a sharp decrease in the inelastic mean free path at the SO phonon energy $E_{SO}$ at which the emission of plasmonlike mode is turned on and an electron loses its energy significantly. Thus, by injecting an electron...
below or above $E_{SO}$, we can change the mean free path of the system significantly, which can be used for designing a lateral hot electron transistor device in the coupled monolayer graphene system.\textsuperscript{22,23} Figure 4(b) shows the inelastic mean free path for bilayer graphene systems. Unlike monolayer graphene, the mean free path in bilayer graphene is much shorter than that in monolayer graphene and the step of the mean free path is very small around $E_{SO}$. Thus the bilayer graphene may not be a good candidate for the application to a lateral hot electron transistor utilizing the electron-phonon interaction. At low energies, however, the inelastic mean free path strongly depends on the carrier density because the threshold energy of the plasmon-like mode $w_-$ is approximately proportional to the Fermi energy. Thus, by changing the carrier density, we can activate or deactivate the decay process via the plasmon-like mode $w_-$ emission, which is possible even in the uncoupled system without SO phonons. With the help of density tunability through gating, we can achieve a significant change in the mean free path. We find that the mean free path of an electron with an energy $\xi_k \approx 0.1$ eV at the carrier density $n \sim 10^{12}$ cm$^{-2}$ is $l \sim 10^2$ nm whereas $l \sim 1 - 10$ nm at $n \sim 10^{11}$ cm$^{-2}$. This promises a possible use of bilayer graphene as a lateral hot electron transistor in the absence of the electron-SO phonon coupling.

IV. DISCUSSION AND SUMMARY

In the previous section we show the self-energy calculated within the dynamical RPA screening. In this section we discuss the effect of dynamical screening of the electron-SO phonon interaction comparing with the results calculated with the static screening. The static screening is equivalent to putting $\omega = 0$ into $\Pi_0(q, \omega)$ in Eq. (7), which means that electrons screen SO phonons statically, while electron-electron interactions are treated dynamically to take into account the plasmon effects.

Figure 5 shows the scattering rates for different carrier densities in monolayer and bilayer graphene with the static or dynamic screening approximation. We find that at low densities the scattering rates with the static screening are larger than those with the dynamic screening for both monolayer and bilayer graphene, while at high densities the results with the dynamic screening are larger than those with the static screening. These effects may arise from the attractive nature of the phonon-mediated effective interaction, which originates from the retardation effect coming from the mass difference between ions and electrons. At low densities, the negative contribution to the scattering rate from the attractive effective interaction is significant, and the static screening suppresses the negative contribution more strongly than the dynamic one, giving larger scattering rate. As the carrier density increases, the negative contribution to the scattering rate becomes negligible, and the scattering rate with the static screening approximation becomes smaller than that with the dynamic screening, as shown in the bottom panel.

In conclusion, we theoretically calculated the inelastic scattering rates $\tau^{-1}$ and the hot electron inelastic mean-free paths $l$ for both monolayer and bilayer graphene on a substrate made of polar materials, treating the electron-electron interaction and the electron-SO phonon interaction on an equal footing. In our theoretical calculation, we include the interaction between electrons, SO phonons, and plasmons within RPA (for dynamical screening and phonon self-energy correction) and within the leading-order self-energy in the effective total interaction. We find that the strong coupling between the SO phonon and plasmon leads to a new decay channel for the quasiparticles through the emission of the coupled mode and gives rise to an abrupt increase in the scattering rate, which is absent in the uncoupled system. In monolayer graphene a single jump in the scattering rate occurs around $E_{SO}$, arising from the emission of the low energy branch of the coupled modes. By varying the energy of an injected electron, we can change the mean free path significantly. In bilayer graphene the emission of both low and high energy branches of the coupled modes contributes to the scattering rate, and gives rise to two abrupt changes in the scattering rate. Especially, in bilayer graphene, the emission of the plasmon-like mode de-
pends strongly on the carrier density while the threshold energy for the emission of the phonon-like mode is weakly dependent on the carrier density and fixed at $E_{SO}$. Utilizing the density dependence of the plasmon-like mode, we can achieve a significant difference in the mean free path by varying the carrier density. With the help of the abrupt changes in $\tau^{-1}$ and $l$ near $E_{SO}$, our results for both monolayer and bilayer graphene are applicable to an electronic device by varying the energy of an injected electron near $E_{SO}$ or tuning the carrier density. It may be possible to fabricate a hot-electron transistor device with a sudden onset of negative differential resistance associated with sharp changes in the inelastic mean free path due to electron-coupled mode scattering of the injected electrons. Especially in monolayer graphene, we note that the sudden sharp changes in the scattering rate occur only when both the electron-electron and electron-SO phonon interactions are considered together, and no such step is obtained with the electron-electron Coulomb interaction alone.\textsuperscript{20}

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