

Lecture Notes on

Low Bias Transport in Graphene: An Introduction

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Abstract - These notes complement a lecture with the same title presented by Mark Lundstrom and Dionisis Berdebes, at the NCN@Purdue Summer School, July 20-24, 2009. That lecture will also be available on www.nanoHUB.org in the “Electronics from the Bottom Up” section (<http://nanohub.org/topics/ElectronicsFromTheBottomUp>)

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1. Introduction

In these notes, we derive some expressions that are useful in understanding low-bias transport in graphene. The notes follow the same structure as the lecture [1]. For every section, they provide proofs and calculations for the expressions that appear in the lecture.

2. Fundamentals of Graphene

2.1) Bandstructure

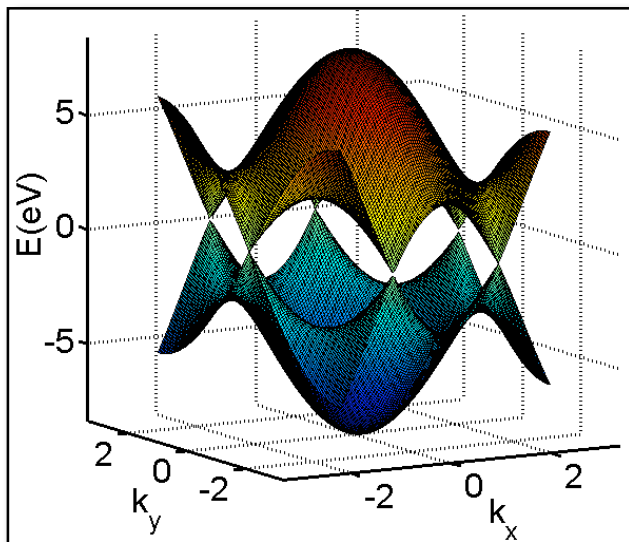


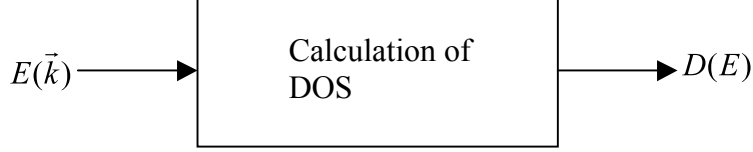
Figure 2.1: Graphene Bandstructure

A thorough discussion on the calculation of the dispersion relation of graphene from its Hamiltonian is available in the following nanoHUB lectures by Professor Datta (course ECE 495N – fall 2008)[13]:

<https://nanohub.org/resources/5710> (Lecture 21)

<https://nanohub.org/resources/5721> (Lecture 22)

2.2) Density of States



The linearized dispersion relation, appropriate for low field transport calculations, is given by

$$E(\vec{k}) = \hbar v_F |\vec{k}|, \quad (2.2.1)$$

where $|\vec{k}|$ is the length of the planar wave vector

$$\vec{k} = (k_x - k_{x0})\vec{x} + (k_y - k_{y0})\vec{y}, \quad (2.2.2)$$

and the point (k_{x0}, k_{y0}) represents the center of one of the six valleys of the graphene dispersion diagram.

We now calculate the density of states using a summation over k space,

$$D(E) = \sum_{\vec{k}} \delta(E - E(\vec{k})) \quad (2.2.3)$$

Changing the summation into an integral, we get

$$D(E) = \frac{WL}{4\pi^2} \int_{-\pi}^{+\pi} d\theta \int_0^{+\infty} k dk \delta(E - E(\vec{k})), \quad (2.2.4)$$

or equivalently

$$D(E) = \frac{WL}{4\pi^2} 2\pi \int_0^{+\infty} \frac{E dE}{(\hbar v_F)^2} \delta(E - E(\vec{k})), \quad (2.2.5)$$

where we have used (2.2.1) to justify the fact that

$$k dk = \frac{E dE}{(\hbar v_F)^2}. \quad (2.2.6)$$

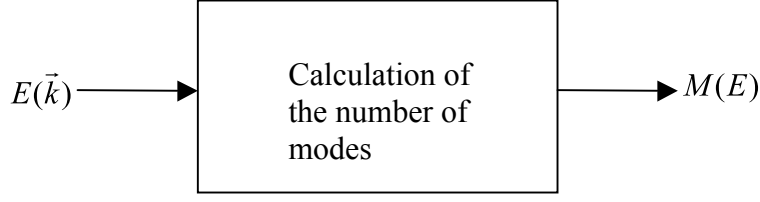
We now use the Dirac function selection rule to obtain

$$D(E) = \frac{WL}{2\pi} \frac{|E|}{(\hbar v_F)^2} \quad (2.2.7)$$

The last step is to include a 2 for the spin and a 2 for the valley degeneracy to get that the DOS for graphene is

$$D(E) = \frac{2WL}{\pi} \frac{|E|}{(\hbar v_F)^2} \quad (2.2.8)$$

2.3) Number of Modes



As before, the graphene dispersion relation is given by

$$E(\vec{k}) = \hbar v_F |\vec{k}| \quad (2.3.1)$$

The number of modes is given as a summation over k space via the following formula

$$M(E) = \sum_{\vec{k}} \delta(E - E(\vec{k})) \frac{\pi \hbar}{L} |v_x(\vec{k})|, \quad (2.3.2)$$

where $v_x(\vec{k})$ is the group velocity in the transport direction x

$$v_x(\vec{k}) = \frac{1}{\hbar} \frac{dE}{dk_x} \quad (2.3.3)$$

Following a similar procedure as before, we obtain

$$\begin{aligned} M(E) &= \frac{WL}{4\pi^2} \frac{\pi \hbar}{L} \int_{-\pi}^{+\pi} d\theta \int_0^{+\infty} k dk \delta(E - E(\vec{k})) \frac{1}{\hbar} \left| \frac{\hbar v_F k_x}{k} \right| \Leftrightarrow \\ M(E) &= \frac{WL}{4\pi} \frac{\pi v_F}{L} \int_{-\pi}^{+\pi} |\cos \theta| d\theta \int_0^{+\infty} k dk \delta(E - E(\vec{k})) \Leftrightarrow \\ M(E) &= \frac{WL}{4\pi} \frac{\pi v_F}{L} \int_0^{+\infty} k dk \delta(E - E(\vec{k})) \Leftrightarrow \\ M(E) &= \frac{W}{\pi} \frac{1}{\hbar v_F} \int_0^{+\infty} E dE \delta(E - E(\vec{k})) \Leftrightarrow \\ M(E) &= \frac{W}{\pi} \frac{|E|}{\hbar v_F} \end{aligned} \quad (2.3.4)$$

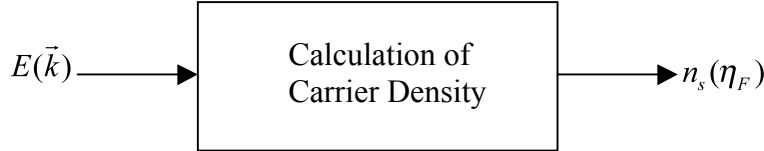
Now, considering also spin degeneracy, we get the final result for the number of conducting channels to be

$$M(E) = \frac{2W}{\pi} \frac{|E|}{\hbar v_F} \quad (2.3.5)$$

2.4) Formula for Transmission

For a derivation of the expression for the transmission function in the Landauer – Büttiker formalism, we refer the reader to Datta, Section 2.2, [14].

2.5) Carrier Density



The net carrier density $n-p$, where n stands for the filled states for $E > 0$, and p for the empty states with $E < 0$, is calculated as the convolution of the density of states with the Fermi Dirac distribution in the energy space.

As already proven before, the density of states per unit energy and volume is given by,

$$D(E) = \frac{2|E|}{\pi(\hbar v_F)^2} \quad (2.5.1)$$

Now, we can proceed to the calculation of carrier density for the general, nonzero T case

$$\begin{aligned} n - p &= \int_0^{+\infty} dE D(E) f(E) - \int_{-\infty}^0 dE D(E) (1 - f(E)) \Leftrightarrow \\ n - p &= \frac{2}{\pi(\hbar v_F)^2} \left(\int_0^{+\infty} dE \frac{E}{1 + e^{(E-E_F)/k_B T}} + \int_{-\infty}^0 dE \frac{E e^{(E-E_F)/k_B T}}{1 + e^{(E-E_F)/k_B T}} \right) \Leftrightarrow \\ n - p &= \frac{2}{\pi(\hbar v_F)^2} \left(\int_0^{+\infty} dE \frac{E}{1 + e^{(E-E_F)/k_B T}} - \int_0^{+\infty} dE \frac{E}{1 + e^{(E+E_F)/k_B T}} \right) \Leftrightarrow \\ n - p &= \frac{2(k_B T)^2}{\pi(\hbar v_F)^2} \Gamma(2) (F_1(\eta_F) - F_1(-\eta_F)) \end{aligned} \quad (2.5.2)$$

The energy space over which the integration is done includes also negative energies, accounting for the valence band of graphene.

Generally, one has to be careful with the Fermi Integral notation,

$$F_s(\eta_F) \equiv \frac{1}{\Gamma(s+1)} \int_0^{\infty} \frac{\varepsilon^s d\varepsilon}{1 + \exp(\varepsilon - \eta_F)} \quad (2.5.3)$$

where

$$F(\eta_F) = \int_0^{\infty} \frac{\varepsilon^s d\varepsilon}{1 + \exp(\varepsilon - \eta_F)} \quad (2.5.4)$$

and $\Gamma(s)$ the Gamma function of order s . For a detailed discussion of Fermi-Dirac integrals, we refer the reader to the notes available on nanohub by Raseong Kim and Mark Lundstrom[15]:

<https://nanohub.org/resources/5475>

The zero temperature approximation is now easy to extract from relation (2.5.2) by making the following substitution,

$$\frac{1}{1 + e^{(E-E_F)/k_B T}} \Big|_{T=0} = 1 - \text{step}(E - E_F), \quad (2.5.3)$$

which will lead to the following

$$n - p = \frac{2}{\pi (\hbar v_F)^2} \left(\int_0^{+\infty} dE E (1 - \text{step}(E - E_F)) - \int_0^{+\infty} dE E (1 - \text{step}(E + E_F)) \right) \quad (2.5.4)$$

or equivalently

$$n - p = \frac{2}{\pi (\hbar v_F)^2} \left(\int_0^{+\infty} \text{pulse}(-E_F, E_F) E dE \right) \quad (2.5.5)$$

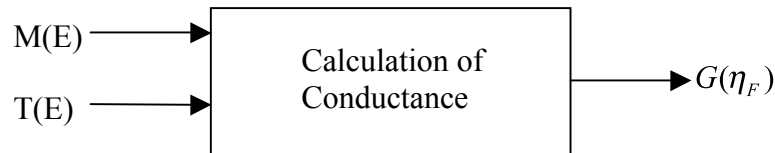
Finally, we get that

$$|n - p| = \frac{E_F^2}{\pi (\hbar v_F)^2}, \quad (2.5.6)$$

which is a simple expression that relates the Fermi energy to the carrier concentration. If we want to account for the sign of the charge of the carrier that is transported in the system, we can rewrite (2.5.5) as

$$n - p = \text{sign}(E_F) \frac{E_F^2}{\pi (\hbar v_F)^2} \quad (2.5.7)$$

2.6) Conductance



In the calculation, we consider two distinct limits:

- Ballistic limit: $T(E) = 1$
- Diffusive limit: $T(E) = \frac{\lambda(E)}{L}$

2.6a) Ballistic limit

The number of conducting channels is

$$M(E) = \frac{2W|E|}{\pi \hbar v_F} \quad (2.6.1)$$

The transmission function is

$$T(E) = 1 \quad (2.6.2)$$

We begin the calculation of conductance from the Landauer formula,

$$G = \frac{2q^2}{h} \int_{-\infty}^{\infty} dE T(E) M(E) \left(-\frac{\partial f_0}{\partial E} \right) \quad (2.6.3)$$

where $-\frac{\partial f_0}{\partial E}$ is equal to

$$-\frac{\partial f_0}{\partial E} = \frac{e^{(E-E_F)/k_B T}}{(1 + e^{(E-E_F)/k_B T})^2} \quad (2.6.4)$$

Introducing (2.6.1), (2.6.2) and (2.6.4) into (2.6.3), we have equivalently

$$G_B = \frac{2q^2}{h} \frac{2W}{\pi \hbar v_F} \left(\int_0^{\infty} dE E \frac{e^{(-E-E_F)/k_B T}}{(1 + e^{(-E-E_F)/k_B T})^2} + \int_0^{\infty} dE E \frac{e^{(E-E_F)/k_B T}}{(1 + e^{(E-E_F)/k_B T})^2} \right) \Leftrightarrow \quad (2.6.5)$$

$$G_B = \frac{2q^2}{h} \frac{2W}{\pi \hbar v_F} \left(\int_0^{\infty} dE E \frac{e^{(E+E_F)/k_B T}}{(1 + e^{(E+E_F)/k_B T})^2} + \int_0^{\infty} dE E \frac{e^{(E-E_F)/k_B T}}{(1 + e^{(E-E_F)/k_B T})^2} \right)$$

Now, noticing that the composite exponential expressions of (2.6.5) can be written as derivatives of Fermi functions with opposite signs for E_F , we can use integration by parts, to obtain

$$G_B = -\frac{2q^2}{h} \frac{2W}{\pi \hbar v_F} \left(\int_0^{\infty} dE E \frac{\partial}{\partial E} \left(\frac{1}{1 + e^{(E+E_F)/k_B T}} \right) - \int_0^{\infty} dE E \frac{\partial}{\partial E} \left(\frac{1}{1 + e^{(E-E_F)/k_B T}} \right) \right) \Leftrightarrow$$

$$G_B = -\frac{2q^2}{h} \frac{2W}{\pi \hbar v_F} \left(-\left[E \frac{1}{1 + e^{(E+E_F)/k_B T}} \right]_0^{\infty} + \int_0^{\infty} dE \frac{1}{1 + e^{(E+E_F)/k_B T}} - \left[E \frac{1}{1 + e^{(E-E_F)/k_B T}} \right]_0^{\infty} + \int_0^{\infty} dE \frac{1}{1 + e^{(E-E_F)/k_B T}} \right) \Leftrightarrow = \quad (2.6.6)$$

$$G_B = \frac{2q^2}{h} \frac{2W}{\pi \hbar v_F} \left(\int_0^{\infty} dE \frac{1}{1 + e^{(E+E_F)/k_B T}} + \int_0^{\infty} dE \frac{1}{1 + e^{(E-E_F)/k_B T}} \right) \Leftrightarrow$$

$$G_B = \frac{2q^2}{h} \frac{2W}{\pi \hbar v_F} (k_B T) (F_0(-\eta_F) + F_0(\eta_F))$$

Now we can yield our final result

$$\boxed{G_B = \frac{2q^2}{h} \frac{2W}{\pi \hbar v_F} (k_B T) \Gamma(1) (F_0(-\eta_F) + F_0(\eta_F))}, \quad (2.6.7)$$

In the zero temperature approximation, $\left(-\frac{\delta f}{\delta E} \right) \approx \delta(E - E_F)$, thus the expression (2.6.3) for conductance, in the ballistic limit, can be reduced to

$$\boxed{G = \frac{2q^2}{h} M(E_F) = \frac{2q^2}{h} \frac{2W |E_F|}{\pi \hbar v_F}}, \quad (2.6.8)$$

according to the Dirac function selection rule.

2.6b) Diffusive Limit

The transmission function is

$$T(E, T) = \frac{\lambda_0(T)}{L} \left(\frac{|E|}{k_B T} \right)^s, \quad (2.6.9)$$

where we assume a mean free path of the form, $\lambda_0(T) \left(\frac{|E|}{k_B T} \right)^s$.

Again, we begin our calculation for conductance from

$$G = \frac{2q^2}{h} \int_{-\infty}^{\infty} dE T(E) M(E) \left(-\frac{\partial f_0}{\partial E} \right) \quad (2.6.10)$$

Now, introducing (2.6.9) and (2.3.5) into (2.6.10) we have

$$G_D = \frac{2q^2}{h} \frac{\lambda_0(T)}{L} \frac{2W}{\pi \hbar v_F} \left(\int_0^{\infty} dE \left(\frac{E}{k_B T} \right)^s E \left(-\frac{\partial f_0}{\partial E} \right) - \int_{-\infty}^0 dE \left(\frac{-E}{k_B T} \right)^s E \left(-\frac{\partial f_0}{\partial E} \right) \right) \quad (2.6.11)$$

We again proceed to the formation of the proper derivatives, in a similar manner to our previous treatment for the ballistic case,

$$G_D = \frac{2q^2}{h} \frac{\lambda_0(T)}{L} \frac{2W}{\pi \hbar v_F} \left(\int_0^{\infty} dE \left(\frac{E}{k_B T} \right)^s E \frac{e^{(E+E_F)/k_B T}}{\left(1 + e^{(E+E_F)/k_B T}\right)^2} + \int_0^{\infty} dE \left(\frac{E}{k_B T} \right)^s E \frac{e^{(E-E_F)/k_B T}}{\left(1 + e^{(E-E_F)/k_B T}\right)^2} \right) \Leftrightarrow \quad (2.6.12)$$

$$G_D = -\frac{2q^2}{h} \frac{\lambda_0(T)}{L} \frac{2W}{\pi \hbar v_F} \left(\int_0^{\infty} dE \left(\frac{E}{k_B T} \right)^s E \frac{\partial}{\partial E} \left(\frac{1}{1 + e^{(E+E_F)/k_B T}} \right) + \int_0^{\infty} dE \left(\frac{E}{k_B T} \right)^s E \frac{\partial}{\partial E} \left(\frac{1}{1 + e^{(E-E_F)/k_B T}} \right) \right)$$

In this general treatment, the integration by parts will not absorb the energy monomial term, but still things don't get too complicated,

$$G_D = \frac{2q^2}{h} \frac{\lambda_0(T)}{L} \frac{2W}{\pi \hbar v_F} \left(\begin{aligned} & - \left[\left(\frac{E}{k_B T} \right)^s E \frac{1}{1 + e^{(E+E_F)/k_B T}} \right]_0^\infty + \\ & + \int_0^\infty dE \left(\frac{s}{k_B T} \left(\frac{E}{k_B T} \right)^{s-1} E + \left(\frac{E}{k_B T} \right)^s \right) \frac{1}{1 + e^{(E+E_F)/k_B T}} \\ & - \left[\left(\frac{E}{k_B T} \right)^s E \frac{1}{1 + e^{(E-E_F)/k_B T}} \right]_0^\infty + \\ & + \int_0^\infty dE \left(\frac{s}{k_B T} \left(\frac{E}{k_B T} \right)^{s-1} E + \left(\frac{E}{k_B T} \right)^s \right) \frac{1}{1 + e^{(E-E_F)/k_B T}} \end{aligned} \right) \Leftrightarrow \\
 G_D = \frac{2q^2}{h} \frac{\lambda_0(T)}{L} \frac{2W}{\pi \hbar v_F} \left(\begin{aligned} & (k_B T) \int_0^\infty dx (s+1) x^s \frac{1}{1 + e^{x+\eta_F}} + \\ & + (k_B T) \int_0^\infty dx (s+1) x^s \frac{1}{1 + e^{x-\eta_F}} \end{aligned} \right) \\
 \boxed{G_D = \frac{2q^2}{h} \frac{\lambda_0(T)}{L} \frac{2W}{\pi \hbar v_F} (k_B T) (s+1) \Gamma(s+1) (F_s(-\eta_F) + F_s(\eta_F))} \quad (2.6.13)$$

In the zero temperature approximation, the diffusive expression for conductance can be reduced to

$$\boxed{G_D = \frac{2q^2}{h} M(E_F) T(E_F) = \frac{2q^2}{h} \frac{2W |E_F|}{\pi \hbar v_F} \frac{\lambda_0(T)}{L} \left(\frac{|E_F|}{k_B T} \right)^s} \quad (2.6.14)$$

Note:

There are restrictions that apply on the value of s . A negative value of the characteristic exponent s will not yield a meaningful calculation, since the diffusive limit assumption will no longer hold for the energy range integrated in the vicinity of zero (mean free path driven to infinity). Thus, one should consider only $s \geq 0$ for a meaningful analytical expression.

3. Experimental Approach

3.1) Gate Voltage – Fermi Energy mapping

The effect of a gate voltage on a graphene-on-substrate system is divided into two parts. A contribution that shifts the Fermi energy level of the system with respect with the dispersion diagram, and a contribution, that changes the carrier concentration within the channel.

The following relation applies

$$V_G = \frac{k_B T}{q} \eta_F + \frac{q}{C_{ox}} n_s(\eta_F) \quad (3.1.1)$$

where

$$n_s(\eta_F) = \left(\frac{2}{\pi}\right) \left(\frac{k_B T}{\hbar v_F}\right)^2 \Gamma(2) (F_1(\eta_F) - F_1(-\eta_F)) \quad (3.1.2)$$

In the experimental literature, people usually assume that $C_{ox}(V_G - V_{NP}) \approx qn_s$, where V_{NP} is the gate voltage at which the minimum of conductance is achieved. This relation implies that the first term of (3.1.1) is too weak to be considered. This approximation is typically robust. In the following plots, we investigate how much the Carrier Density-Gate Voltage relation is affected by the $C_{ox}(V_G - V_{NP}) \approx qn_s$ approximation.

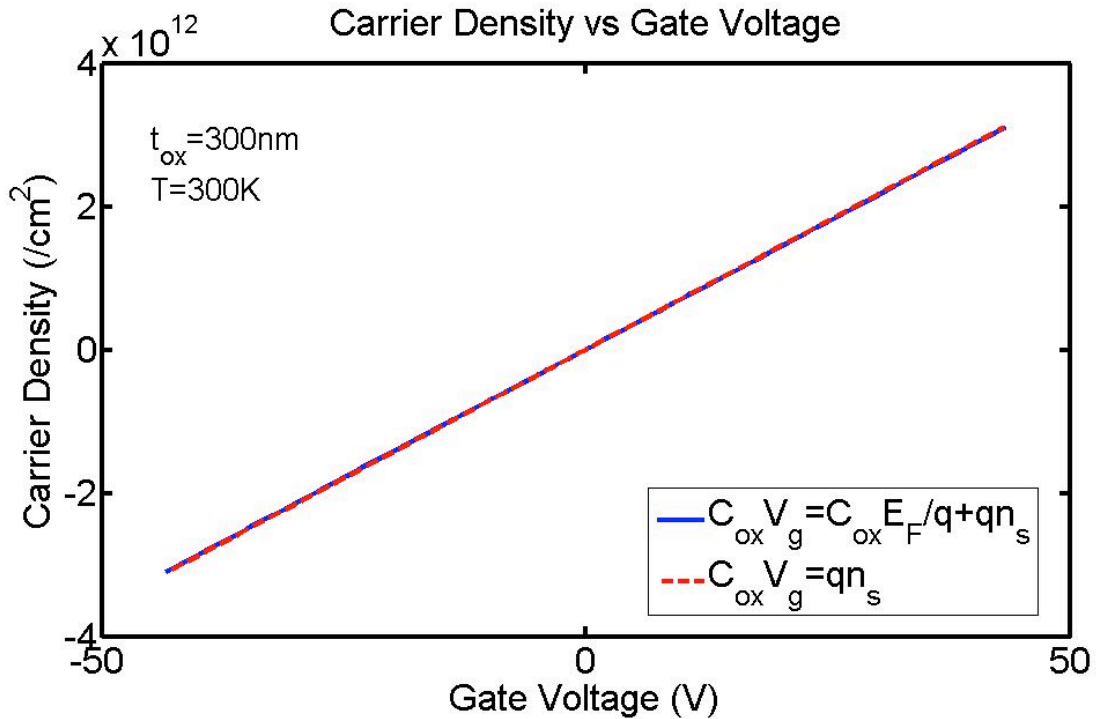


Figure 3.1: Carrier Density vs. Gate Voltage for room temperature and thick oxide.

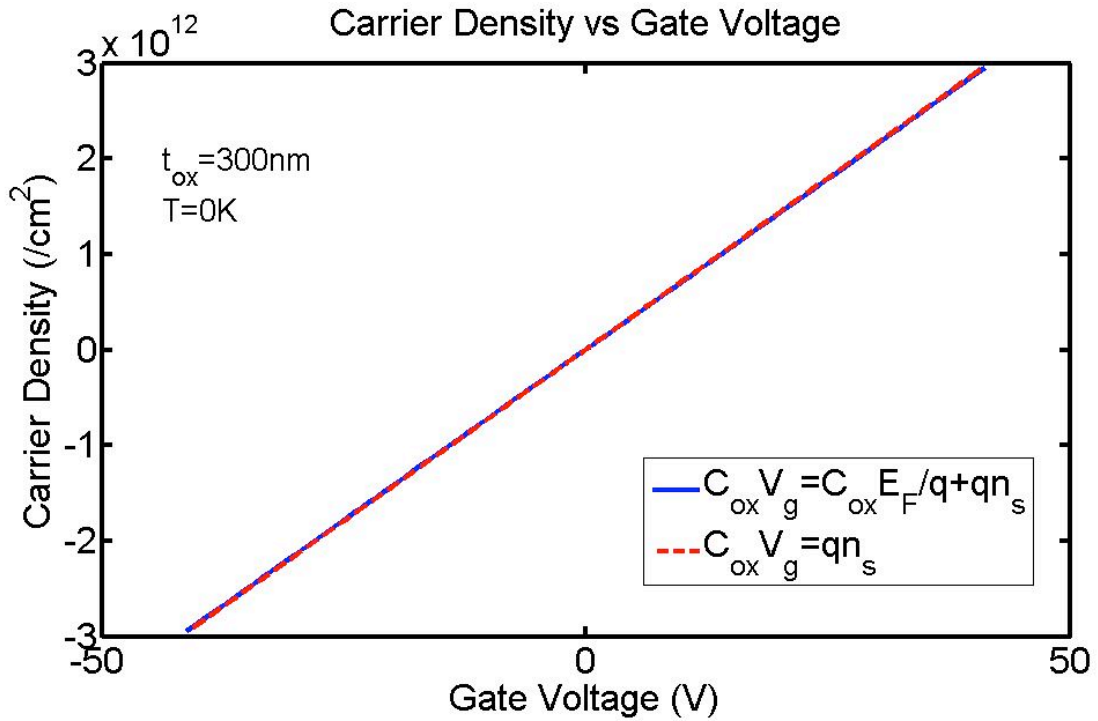


Figure 3.2: Carrier Density vs. Gate Voltage for zero temperature and thick oxide

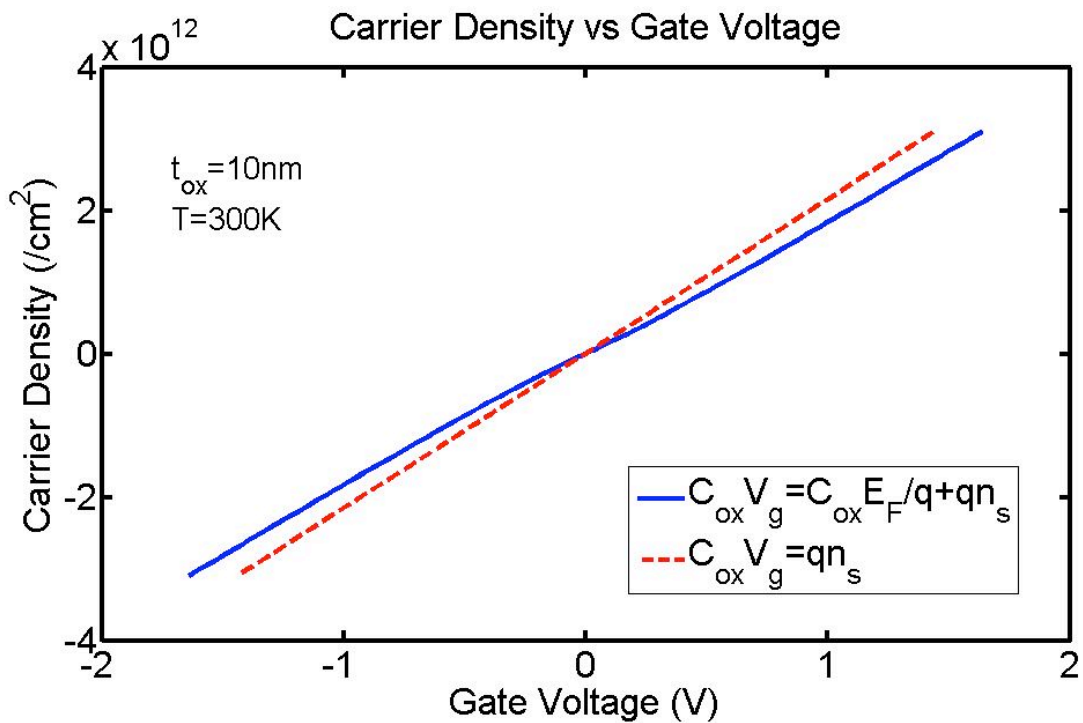


Figure 3.3: Carrier Density vs. Gate Voltage for room temperature and thin oxide

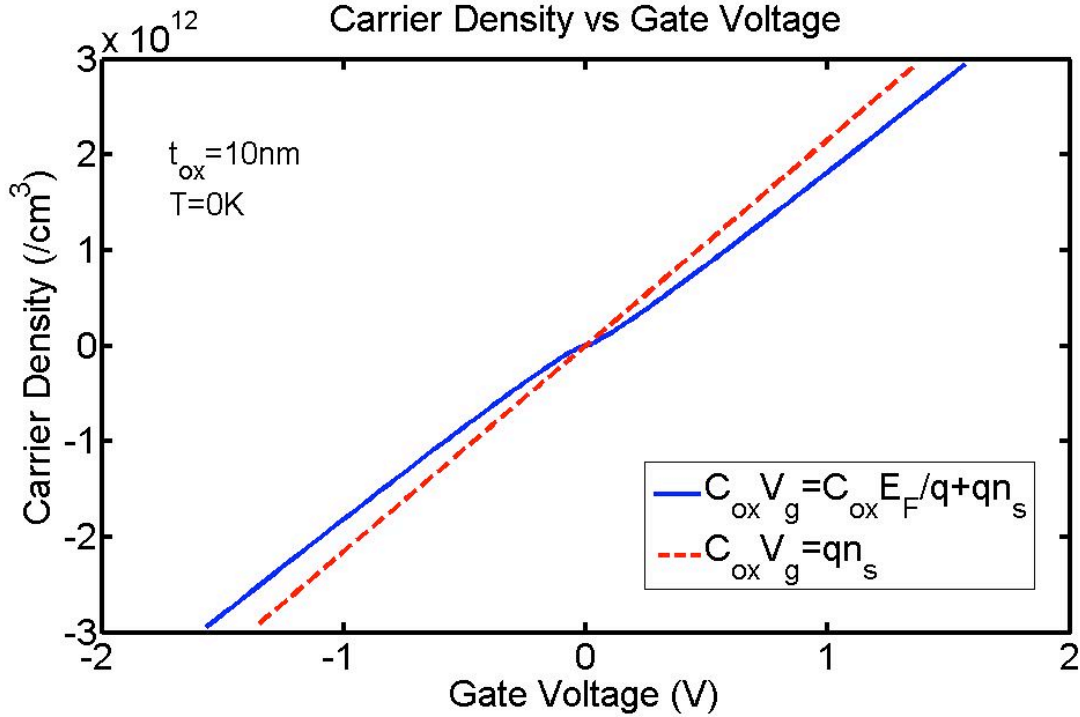
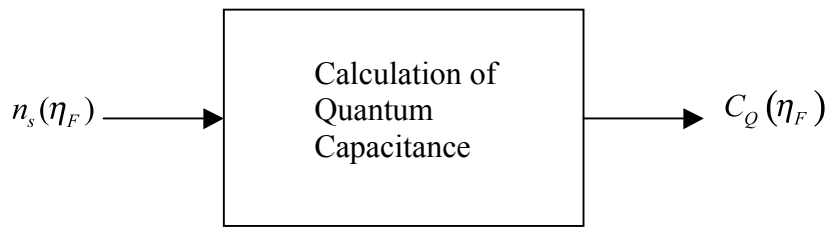


Figure 3.4: Carrier Density vs. Gate Voltage for zero temperature and thin oxide

It is interesting to note, that the assumption generally made in the experimental literature, performs well. It remains valid over a large range of temperatures, but it breaks down for very small oxide thicknesses. For 90 nm or 300 nm, which are the typical thicknesses, however, one can assume that $C_{ox} (V_G - V_{NP}) \approx qn_s$ with confidence.

3.2) Quantum Capacitance



Central to the discussion in section 3.1 is the concept of quantum capacitance. The quantum capacitance of a carrier density is calculated as the derivative of carrier density vs. energy at the Fermi energy,

$$C_Q(E_F) = q^2 \left[\frac{dn}{dE} \right]_{E=E_F} \quad (3.2.1)$$

In addition, the electron concentration is related to the Fermi energy as follows

$$n_s(\eta_F) = \left(\frac{2}{\pi} \right) \left(\frac{k_B T}{\hbar v_F} \right)^2 \Gamma(2) (F_1(\eta_F) - F_1(-\eta_F)) \quad (3.2.2)$$

Thus

$$\left. \frac{dn}{dE} \right|_{E=E_F} = \frac{2k_B T}{\pi (\hbar v_F)^2} \Gamma(2) (F_0(\eta_F) + F_0(-\eta_F)) \quad (3.2.3)$$

Now, the quantum capacitance can be extracted

$$C_Q(E_F) = \frac{2k_B T q^2}{\pi (\hbar v_F)^2} \Gamma(2) (F_0(\eta_F) + F_0(-\eta_F)) \quad (3.2.4)$$

4. Results

4.1) Sheet Conductance for $E_F = 0$

The general expression for conductance for a single principal scattering mechanism, at the diffusive limit, has been derived to be (2.6.14)

$$G_D = \frac{2q^2}{h} \frac{\lambda_0(T)}{L} \frac{2W}{\pi \hbar v_F} (k_B T)(s+1) \Gamma(s+1) (F_s(-\eta_F) + F_s(\eta_F)) \quad (4.1.1)$$

We can write the conductance as

$$G_D = \sigma_D \frac{W}{L} \quad (4.1.2)$$

From (4.1.1) and (4.1.2), one can yield the sheet conductance vs η_F to be

$$\sigma_D = \frac{2q^2}{h} \lambda_0(T) \frac{2}{\pi \hbar v_F} (k_B T)(s+1) \Gamma(s+1) (F_s(-\eta_F) + F_s(\eta_F)), \quad (4.1.3)$$

It is interesting to focus on what the Landauer theory predicts for the minimum sheet conductance. In particular, if we substitute $E_F = 0$, we get

$$\sigma_D = \frac{2q^2}{h} \frac{2}{\pi \hbar v_F} (k_B T)(s+1) \Gamma(s+1) F_s(0) \lambda_0(T) \quad (4.1.4)$$

where s is the characteristic exponent of the principal scattering mechanism as defined in (2.6.9). Please note that we can recover the ballistic conductivity at the minimum by substituting $s = 0$ and $\lambda_0(T) = L$.

4.2) Calculation details of slides 24-27

The temperature of the system is $T = 10K$. It is possible to assume the zero-T approximation for both the $n_s/V_g/E_f$ relation and for the expression for conductance. In addition, the linear behavior of conductivity vs gate voltage suggests strong presence of scattering with mean free path with characteristic exponent $s=1$. Thus, we can write down:

$$n_s = \left(\frac{1}{\pi} \right) \left(\frac{E_F}{\hbar v_F} \right)^2 \quad (4.2.1)$$

$$C_{ox} (V_G - V_{NP}) = qn_s \quad (4.2.2)$$

$$C_{ox} = \frac{\epsilon_{SiO_2}}{t_{ox}} \quad (4.2.3)$$

$$\sigma_D(E_F) \approx \frac{2q^2}{h} \lambda(E_F) \left(\frac{2E_F}{\pi \hbar v_F} \right) \quad (4.2.4)$$

From (4.2.1-3), one can derive the Fermi energy from a given gate voltage value ($V_g = 50, 100V$). Then, taking the values for conductivity at these voltages and using (4.2.4) one can calculate $\lambda(E_F)$.

Please note that for this particular sample, the linearity of sheet conductance vs. carrier concentration/gate voltage should suggest a mobility that is independent of carrier density.

5. Analysis

5.1 Definition of mean-free-path for backscattering - Landauer Approach vs. the Boltzmann Transport Equation Approach

For diffusive transport, the conductance is frequently computed by solving the Boltzmann transport equation, so the question arises as to how the two approaches compare with each other. From the Landauer approach for graphene in the diffusive limit at $T = 0K$, we have

$$G = \left(\frac{2q^2}{h} \right) \left(\frac{2E_F}{\pi \hbar v_F} \right) \lambda(E_F) \left(\frac{W}{L} \right) \quad (5.1.1)$$

or

$$\sigma_D = \left(\frac{2q^2}{h} \right) \left(\frac{2E_F}{\pi \hbar v_F} \right) \lambda(E_F) \quad (5.1.2)$$

How does this compare to the result obtained by solving the BTE? Begin with the steady-state BTE without density gradient (Lundstrom, 3.2 [2])

$$-qE_x \frac{\partial f}{\partial p_x} = - \left. \frac{\partial f}{\partial t} \right)_{coll} \quad (5.1.3)$$

Assuming the Relaxation Time Approximation (RTA) for the collision integral (Lundstrom, 3.3.2 [2]), this equation becomes

$$-qE_x \frac{\partial f}{\partial p_x} = \frac{(f - f_0)}{\tau_f} = - \frac{f_1}{\tau_f} \quad (5.1.4)$$

which is valid for isotropic or elastic scattering with τ_f then being the momentum relaxation time [2]. Assuming a voltage drop of V across a resistor of length L , we use the chain rule for the derivative

$$-q \left(-\frac{V}{L} \right) \frac{\partial f}{\partial E} \frac{\partial E}{\partial p_x} = - \frac{f_1}{\tau_f} \quad (5.1.5)$$

which can be solved to find

$$f_1 = q\tau_f v_x \left(-\frac{\partial f}{\partial E} \right) \frac{V}{L} \quad (5.1.6)$$

The current per unit width is evaluated from

$$\frac{I}{W} = \frac{1}{A} \sum_{\vec{k}} q v_x f_1 \quad (5.1.7)$$

Converting the sum to an integral,

$$\frac{I}{W} = \frac{1}{A} \sum_{\vec{k}} q v_x f_1 = \left\{ \frac{1}{A} \frac{A}{(2\pi)^2} 2 \times 2 \times \int_{-\pi/2}^{+\pi/2} d\theta \int_0^{\infty} k dk q^2 v_x^2 \tau \left(-\frac{\partial f_0}{\partial E} \right) \right\} \frac{V}{L} \quad (5.1.8)$$

The first factor of 2 is for spin and the second is for valley degeneracy. Using $v_x = v_F \cos \theta$, we find

$$\frac{I}{W} = \left\{ \frac{1}{\pi^2} \int_0^{2\pi} \cos^2 \theta d\theta \int_0^{\infty} k dk q^2 v_F^2 \tau \left(-\frac{\partial f_0}{\partial E} \right) \right\} \frac{V}{L} \quad (5.1.9)$$

The integral over k can be converted to an integral over energy using the dispersion (i.e. $E(k)$) for graphene

$$E = \hbar v_F k \rightarrow k dk = \frac{E dE}{(\hbar v_F)^2} \quad (5.1.10)$$

to find

$$\frac{I}{W} = \left\{ \frac{1}{\pi} \int_0^{\infty} \frac{E dE}{(\hbar v_F)^2} q^2 v_F^2 \tau \left(-\frac{\partial f_0}{\partial E} \right) \right\} \frac{V}{L} \quad (5.1.11)$$

from which we find

$$\sigma_D = \frac{1}{\pi} \int_0^{\infty} \frac{E dE}{(\hbar v_F)^2} q^2 v_F^2 \tau_f \left(-\frac{\partial f_0}{\partial E} \right) \quad (5.1.12)$$

at $T = 0\text{K}$,

$$\left(-\frac{\partial f_0}{\partial E}\right) = \delta(E - E_F) \quad (5.1.13)$$

so the integral becomes

$$\sigma_D = \frac{1}{\pi} \frac{E_F}{(\hbar v_F)^2} q^2 v_F^2 \tau_f(E_F) \quad (5.1.14)$$

which can be written as

$$\sigma_D = \frac{2q^2}{h} \frac{E_F}{\pi \hbar v_F} \left(\frac{\pi}{2} v_F \tau_f(E_F)\right) \quad (5.1.15)$$

which is exactly eqn. (5.1.2) from the Landauer approach provided we define the “mean-free-path” for backscattering to be

$$\boxed{\lambda(E_F) \equiv \frac{\pi}{2} v_F \tau_f(E_F)} \quad (5.1.16)$$

Finally, note that the BTE result (5.1.14) is often written in another way. Recall that the density of states for graphene is

$$D(E) = \frac{2|E|}{\pi(\hbar v_F)^2} \quad (5.1.17)$$

so eqn. (5.1.14) can be written as

$$\sigma_D = q^2 D(E) \frac{v_F^2}{2} \tau_f(E_F) \quad (5.1.18)$$

or recognizing the diffusion coefficient for electrons at energy, E , as

$$D_n(E) = \frac{v_F^2}{2} \tau_f(E_F) \quad (5.1.19)$$

we can write the sheet conductance from the BTE as

$$\boxed{\sigma_D = q^2 D(E) D_n(E)} \quad (5.1.20)$$

which is true in general, not just for graphene.

5.2 Extraction of the apparent mean-free-path from experimental data

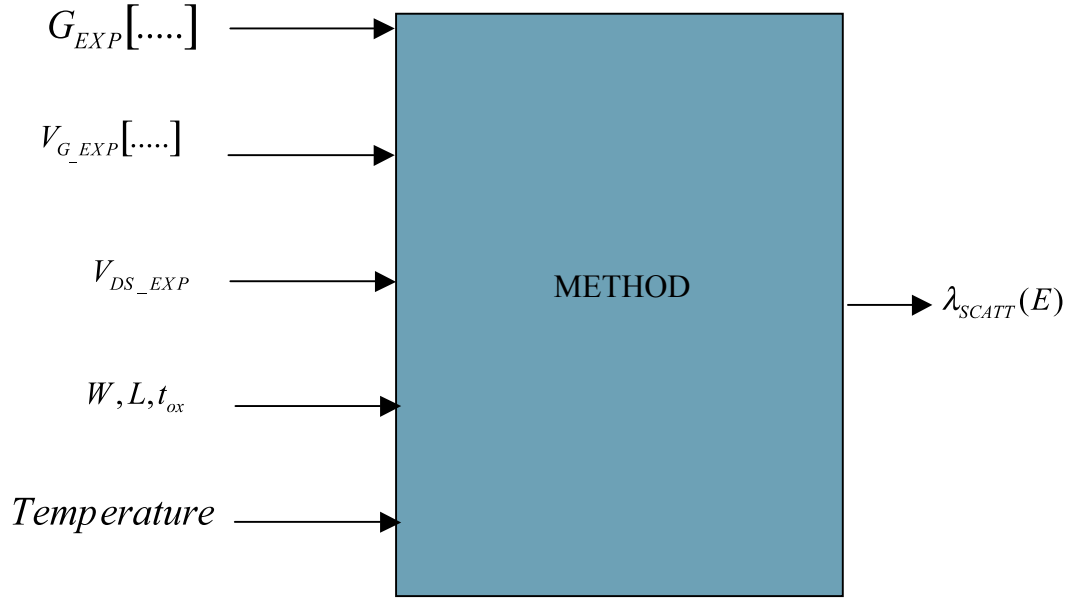


Figure 5.1: Inputs and outputs of experimental data analysis

As it can be seen in the schematic, in the analysis of experimental data, we need the dimensions of the system, the temperature of the environment, the applied voltages and the measured conductance.

In the extraction of the mean free path, we assume a zero temperature approximation. In this case, we have

$$G(0K) = \frac{2q^2}{h} T(E_F) M(E_F) = \left\{ \frac{4q^2}{h} \frac{E_F}{\pi \hbar v_F} \frac{\lambda(E_F)L}{\lambda(E_F)+L} \right\} \frac{W}{L} = \sigma_D \frac{W}{L}, \quad (5.2.1)$$

or for the sheet conductance

$$\sigma_D = \left\{ \frac{4q^2}{h} \frac{E_F}{\pi \hbar v_F} \frac{\lambda(E_F)L}{\lambda(E_F)+L} \right\}. \quad (5.2.2)$$

We now define an apparent mean free path

$$\boxed{\lambda_{app} \triangleq \frac{\lambda(E_F)L}{\lambda(E_F)+L}}, \quad (5.2.3)$$

which is equivalent to writing

$$\frac{1}{\lambda_{app}} = \frac{1}{\lambda(E_F)} + \frac{1}{L} \quad (5.2.4)$$

The relation between sheet conductance and conductance was discussed also in section 4.1. In this section, however, the difference between the mean free path and the apparent mean free path is clarified. This need didn't arise in 4.1, because at the diffusive limit, $\lambda \approx \lambda_{app}$.

Now, one can extract a zero temperature approximation apparent mean free path that depends on Fermi energy as follows

$$\lambda_{app}(E_F) = \frac{\sigma_D}{\frac{4q^2 E_F}{h \pi \hbar v_F}} \quad (5.2.5)$$

Usually, one has experimental input of the form $\sigma_D(n_s)$, thus one might also use (4.2.1) to get

$$\lambda_{app}(V_g) = \frac{\sigma_D(V_g)}{4q^2 \sqrt{n_s(V_g)} \pi / h} \quad (5.2.6)$$

Now, we can recover the mean free path to be compared with scattering theory with the use of (5.2.4), if we know the length of the sample.

6. Electron Scattering in Graphene

The measured conductance of graphene depends on the microscopic scattering processes that occur. This is still an active field of research. In these notes, we only wish to review some of the major features of scattering in graphene and to discuss briefly how scattering rates are computed.

6.1 Important scattering mechanisms in graphene

Identifying the major scattering mechanisms limiting the transport properties of graphene is important from a device point of view. In this section, we shall review some of the commonly known scattering mechanisms believed to be playing an important role in graphene.

Short range scattering potential due to localized defects has been discussed in the literature [3,11,12], where one usually approximate the scattering potential by a delta function. The important point is that short range scattering potentials give rise to a scattering time (and mean-free-path) that varies as $1/E$ and is independent of temperature.

Charged impurity scattering is thought to be an important scattering mechanism in graphene [7]. For unscreened Coulomb scattering, one finds [3,8] that $\tau(E) \propto E$, which leads to a conductance that is proportional to n_s . In practice, we expect the charges to be screened by the carriers in the graphene. In fact, the observation of a linear conductance vs. n_s characteristic is frequently taken as evidence for the presence of charged impurity scattering. It has been pointed out, however, that uncharged defects can also lead to this behavior, if the scattering potential is strong enough to induce mid-gap states [9]. Recent experimental studies on intentionally damaged graphene have shown that strong defect scattering can produce linear conductance vs. n_s .

Deformation potential scattering by acoustic phonons [4,9] is also believed to be an important scattering mechanism. The precise value of D_A is uncertain with values from 10-30 eV being reported [4]. Optical phonons in the graphene can also scatter carriers – especially at temperatures above 300K [5]. Some authors believe that optical phonon in graphene are responsible for the decrease in conductivity at high temperatures [5] while others feel that polar optical phonon in the underlying SiO₂ are responsible [6].

6.2 Deriving relaxation time in graphene: an example

In this section, we illustrate how to derive the momentum relaxation time in graphene. We shall consider the deformation potential (ADP) scattering as an example. The main physics follow the classic approach described in [2], pp. 64-67, 73-82). The only modification that one made to this simple approach [2] is to account for the fact that the graphene wavefunction is described by a two-component wavefunction as follows:

$$\Psi(\vec{k}) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ e^{i\theta} \end{pmatrix} e^{i\vec{k}\cdot\vec{r}} \quad (6.2.1)$$

where

$$e^{i\theta} = \frac{k_x + ik_y}{k} \quad (6.2.2)$$

This arises from the property of the linear dispersion relationship of graphene. The overlap between two plane waves is

$$\int \Psi'(\vec{k}') \Psi(\vec{k}) d\vec{r} = \frac{1}{2} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ e^{i\theta} \end{pmatrix} = \frac{1}{2} (1 + e^{i\theta}) \quad (6.2.3)$$

This then yields us the overlap probability

$$\left| \int \Psi'(\vec{k}') \Psi(\vec{k}) d\vec{r} \right|^2 = \frac{1}{4} (1 + e^{i\theta})(1 + e^{-i\theta}) = \frac{1}{2} (1 + \cos\theta) \quad (6.2.4)$$

We first identify the perturbing potential as ([2], p. 60- 61)

$$U_S(r) = D_A \nabla u_\beta \quad (6.2.5)$$

Writing the Fourier components of the acoustic wave as

$$u_\beta = A_\beta e^{\pm i\vec{\beta}\cdot\vec{r}} e^{i\omega_\beta t} \quad (6.2.6)$$

and inserting the result in eqn. (15), we find

$$U_S(r) = \beta D_A u_\beta \quad (6.2.7)$$

We wish to described the transition rate (probability per second) for scattering from the incident state, \vec{k} , to the final state, \vec{k}' . This is usually done using first order perturbation theory (Fermi's Golden Rule) as ([2], pp. 41-46)

$$S(k, k') = \frac{2\pi}{\hbar} |H_{k'k}|^2 \delta(E' - E - \Delta E) s^{-1} \quad (6.2.8)$$

where the matrix element is

$$H_{k'k} = \int \psi_{k'}^*(r) U_S(r) \psi_k(r) d^2r \quad (6.2.9)$$

The energy of the scattered electron is

$$E' = E + \Delta E \quad (6.2.10)$$

where $E' = E + \Delta E$ is the change in energy as a result of scattering (zero for elastic scattering). Static potentials cause elastic scattering, and time-varying potentials describe inelastic scattering.

For acoustic phonons, the scattering potential is simply a constant with respect to the integration variables in (6.2.9). So we can write Eq. (6.2.8) as

$$S(k, k') = \frac{2\pi}{\hbar} \left[\frac{1}{2} (1 + \cos \theta) \right] (\beta D_A A_\beta)^2 \delta_{k', k \pm \beta} \delta(E' - E) \quad (6.2.11)$$

where, following the arguments in [2] (pp.73-74), we have assumed that acoustic phonon scattering near room temperature is elastic. In this expression, the Kronecker delta expresses momentum conservation, and the delta function, energy conservation.

Next, we must quantize the lattice vibrations by replacing the magnitude of the classical wave in (6.2.6) by its quantum mechanical counterpart (see [2], pp. 77-78)

$$|A_\beta|^2 \rightarrow \frac{\left(N + \frac{1}{2} \mp \frac{1}{2} \right) \hbar}{2M\omega_\beta} \quad (6.2.12)$$

Where the top sign denotes acoustic phonon emission and the bottom sign, absorption. The number of acoustic phonons is give by the Bose-Einstein occupation factor

$$N = \frac{1}{e^{\hbar\omega/k_B T} - 1} \quad (6.2.13)$$

For a typical acoustic phonon involved in electron-phonon scattering, $\hbar\omega < k_B T$ ([2], pp. 73-74), so we can expand the exponential in (6.2.13) and find

$$N \approx \frac{k_B T}{\hbar\omega_\beta} \gg 1 \quad (6.2.14)$$

As a result of 6.2.14, we find

$$\left(N + \frac{1}{2} \mp \frac{1}{2} \right) \approx N \quad (6.2.15)$$

So we can just sum the absorption and emission rates. Returning to (6.2.12), M is the total mass within the normalization area, A ,

$$M = \rho_m A \quad (6.2.16)$$

For small wave-vector, β , the acoustic phonon dispersion is linear ([2], pp. 46-48), so

$$\frac{\omega_\beta}{\beta} = v_s = \sqrt{\frac{c_l}{\rho_m}} \quad (6.2.17)$$

Since these are the low energy phonons involved in elastic ADP scattering, we can use 6.2.17 along with eqns. (6.2.11-15) in the expression for the transition rate, (6.2.80) to find

$$\begin{aligned} S(k, k') &= \frac{2\pi}{\hbar} \left[\frac{1}{2} (1 + \cos \theta) \right] (\beta D_A A_\beta)^2 \delta_{k', k \pm \beta} \delta(E' - E) \Leftrightarrow \\ S(k, k') &= \frac{2\pi}{\hbar} \left[\frac{1}{2} (1 + \cos \theta) \right] \frac{D_A^2 \omega_\beta^2}{v_s^2} \frac{N_\beta \hbar}{\rho_m A \omega_\beta} \delta_{k', k \pm \beta} \delta(E' - E) \Leftrightarrow \\ S(k, k') &= \frac{2\pi}{\hbar} \left[\frac{1}{2} (1 + \cos \theta) \right] \left(\frac{D_A^2 \hbar \omega_\beta}{\rho_m A v_s^2} \right) N_\beta \delta_{k', k \pm \beta} \delta(E' - E) \end{aligned} \quad (6.2.18)$$

From the transition rate, we find the total scattering rate as

$$\begin{aligned} \frac{1}{\tau_m(E)} &= \sum_{k'} (1 - \cos \theta) S(k, k') \\ &= \frac{2\pi}{\hbar} \left(\frac{D_A^2 \hbar \omega_\beta}{\rho_m A v_s^2} \right) N_\beta \sum_{k'} \left[\frac{1}{2} (1 + \cos \theta) \right] (1 - \cos \theta) \delta(E' - E) \\ &= \frac{2\pi}{\hbar} \left(\frac{D_A^2 \hbar \omega_\beta}{\rho_m A v_s^2} \right) N_\beta \frac{A}{(2\pi)^2} \frac{1}{2} \frac{k}{\hbar v_f} \int_0^{2\pi} (1 + \cos \theta)(1 - \cos \theta) d\theta \\ &= \frac{2\pi}{\hbar} \left(\frac{D_A^2 \hbar \omega_\beta}{\rho_m v_s^2} \right) N_\beta \frac{E\pi}{2(2\pi\hbar v_f)^2} = \frac{2\pi}{\hbar} \left(\frac{D_A^2 k_B T}{\rho_m v_s^2} \right) \frac{E\pi}{2(2\pi\hbar v_f)^2} \\ &= \frac{D_A^2 k_B T E}{4\hbar^3 \rho_m v_f^2 v_s^2} \end{aligned} \quad (6.2.19)$$

We arrive at the same result as [4,9]. According to [4], the acoustic deformation potential for graphene is $D_A = 18 \pm 1$ eV, the velocity of LA phonons is $v_s = 2.1 \times 10^6$ cm/s, and the mass density is $\rho = 7.6 \times 10^{-7}$ kg m⁻².

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