NCN Summer School: July 2011

Near-equilibrium Transport:
Fundamentals and Applications

Lecture 10: Case Study: Graphene

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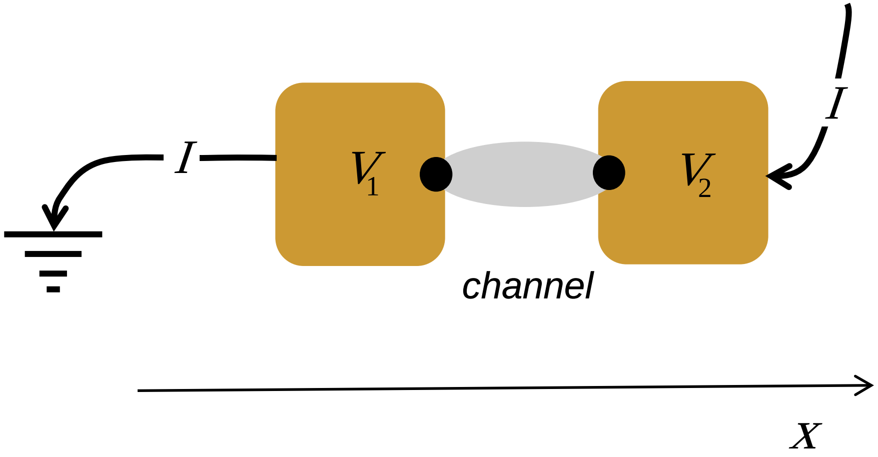
review

$$I = G(\Delta V + S\Delta T)$$

$$I_Q = -T_L S G \Delta V - K_0 \Delta T$$



$$G = \int G'(E)\,dE$$

$$S = \frac{-\int \frac{(E-E_F)}{qT_L} G'(E)\,dE}{\int G'(E)\,dE}$$

$$K_0 = \int \frac{(E-E_F)^2}{q^2 T_L} G'(E)\,dE$$

$$G'(E) = \frac{2q^2}{h} T(E) M(E) \left(-\frac{\partial f_0}{\partial E}\right)$$

diffusive transport in 2D

$$J_x = \sigma\left(\frac{d\left(F_n/q\right)}{dx} - S\frac{dT_L}{dx}\right)$$

$$J_x^q = -\pi\sigma\frac{d\left(F_n/q\right)}{dx} - \kappa_0\frac{dT_L}{dx}$$

$$\frac{d\left(F_n/q\right)}{dx} = \rho J_x + S\frac{dT_L}{dx}$$

$$J_x^q = \pi J_x - \kappa_e\frac{dT_L}{dx}$$

$$\sigma_n = \int \sigma'(E)\,dE$$

$$\sigma'(E) = \frac{2q^2}{h}\lambda(E)\frac{M(E)}{W}\left(-\frac{\partial f_0}{\partial E}\right)$$

$$S = -\int \frac{\left(E - E_F\right)}{qT_L}\sigma'(E)\,dE \Big/ \sigma$$

$$\pi = T_L S$$

$$\kappa_0 = \int \frac{\left(E - E_F\right)^2}{q^2 T_L}\sigma'(E)\,dE$$

$$\kappa_e = \kappa_0 - \pi S\sigma$$

evaluating the transport parameters

Only two quantities are needed: $M(E)$ and $T(E)$ or $\lambda(E)$

For a 2D conductor with **parabolic energy bands**:

$$M_{2D}(E) = W M_{2D}(E) = W \frac{\sqrt{2m^*(E - E_C)}}{\pi\hbar}$$

For a 1D or 2D conductor with parabolic energy bands $M(E)$ is given by different expressions. $T(E)$ depends on dimensionality and the particular scattering mechanisms that dominate.

nonparabolic energy bands in 1D, 2D, or 3D

What if the bandstructure is non-parabolic?

Graphene is a good example, because $E(k)$ is simple, but distinctly non-parabolic. It is also a material that is of great interest currently.

2011 Nobel Prize in Physics

The Nobel Prize in Physics 2010
Andre Geim, Konstantin Novoselov

Photo: U. Montan
Andre Geim

Photo: U. Montan
Konstantin Novoselov

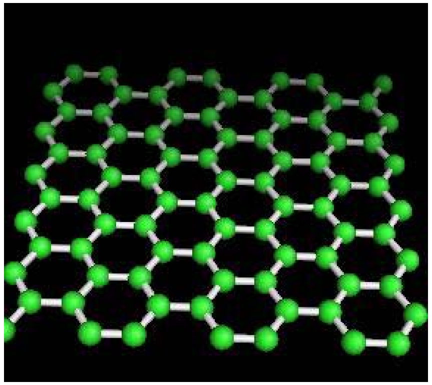
The Nobel Prize in Physics 2010 was awarded jointly to Andre Geim and Konstantin Novoselov *"for groundbreaking experiments regarding the two-dimensional material graphene"*

"The Nobel Prize in Physics 2010". Nobelprize.org. 9 Jun 2011
http://nobelprize.org/nobel_prizes/physics/laureates/2010/

outline

graphene

Graphene is a one-atom-thick planar carbon sheet with a honeycomb lattice.



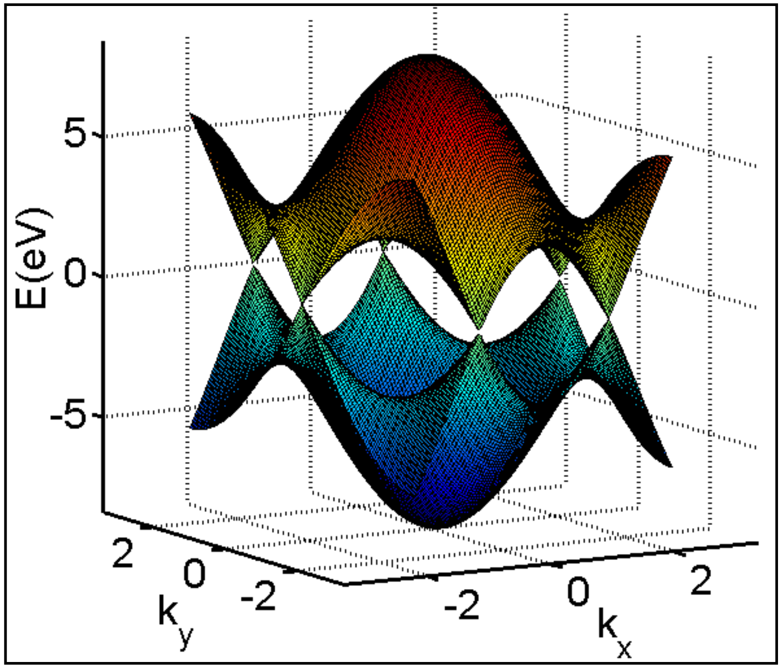
source: CNTBands 2.0 on nanoHUB.org

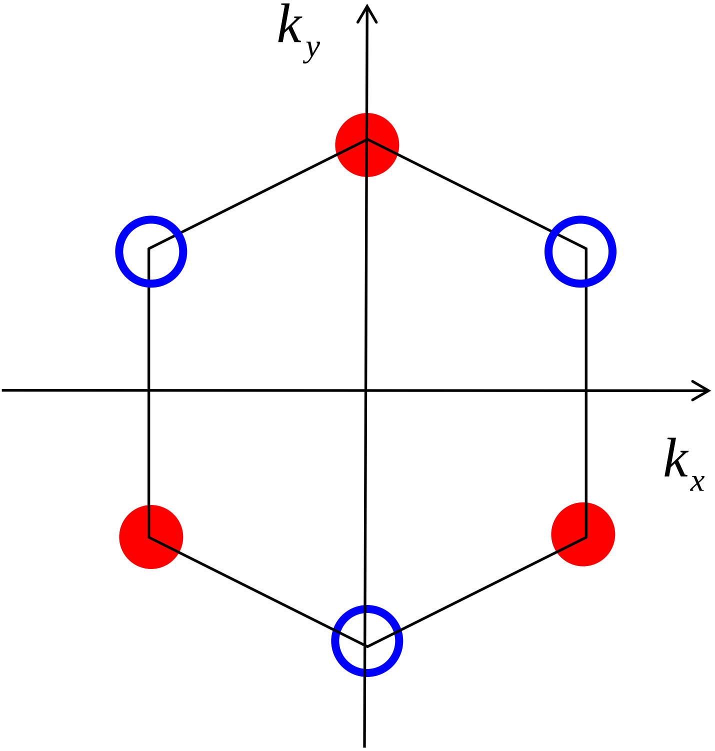
Graphene has an unusual bandstructure that leads to interesting effects and potentially to useful electronic devices.

graphene bandstructure

E(*k*)

Brillouin zone

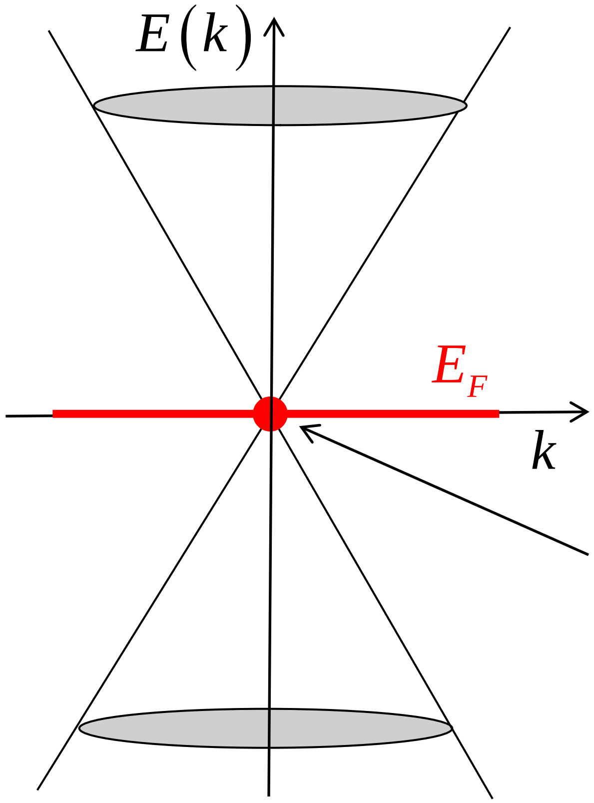




Datta: ECE 495N – fall 2008:
https://nanohub.org/resources/5710 (Lecture 21)
https://nanohub.org/resources/5721 (Lecture 22)

simplified graphene bandstructure near *E* = 0

We will use a very simple description of the graphene bandstructure, which is a good approximation near the Fermi level.



$$E(k) = \pm\hbar\upsilon_F k = \pm\hbar\upsilon_F\sqrt{k_x^2 + k_y^2}$$

$$\upsilon(k) = \frac{1}{\hbar}\frac{\partial E}{\partial k} = \upsilon_F$$

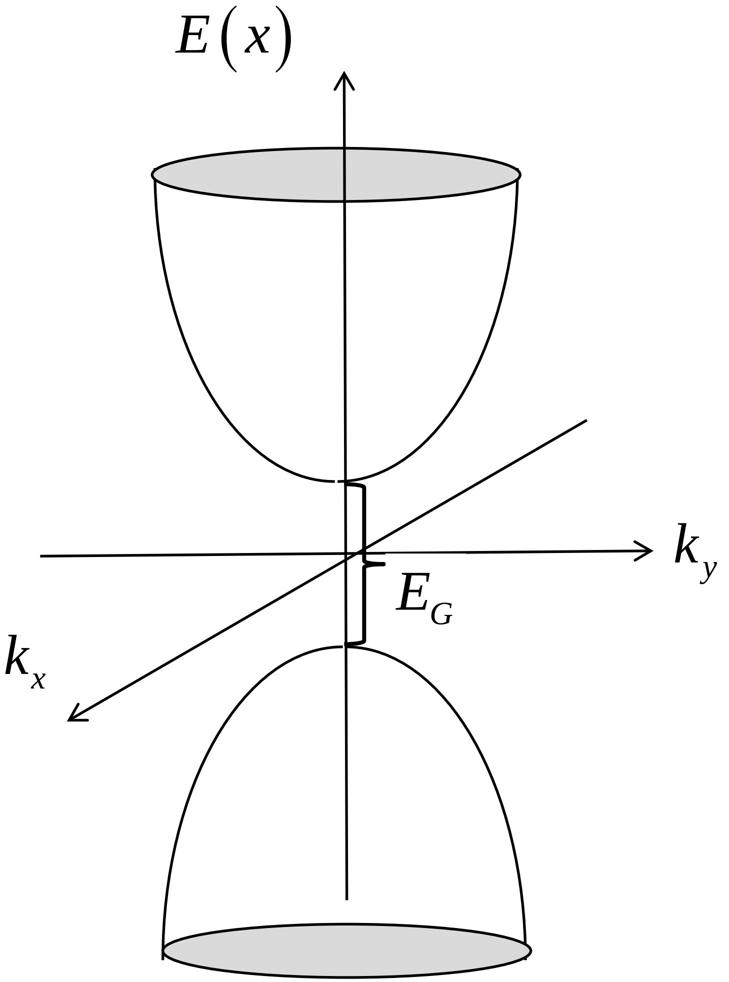
$$\upsilon(k) = \upsilon_F \approx 1\times 10^{8}\,\mathrm{cm/s}$$

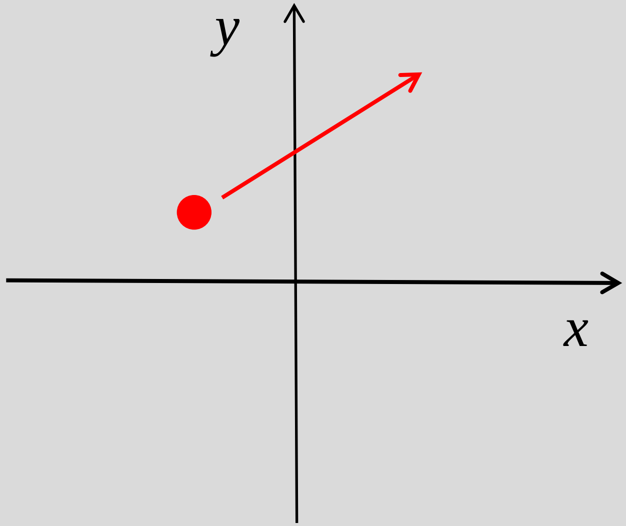
$g_V = 2$ (valley degeneracy)

"neutral point" ("Dirac point")

We will refer to the $E_F > 0$ case, as "n-type graphene" and to the $E_F < 0$ case as "p-type graphene."

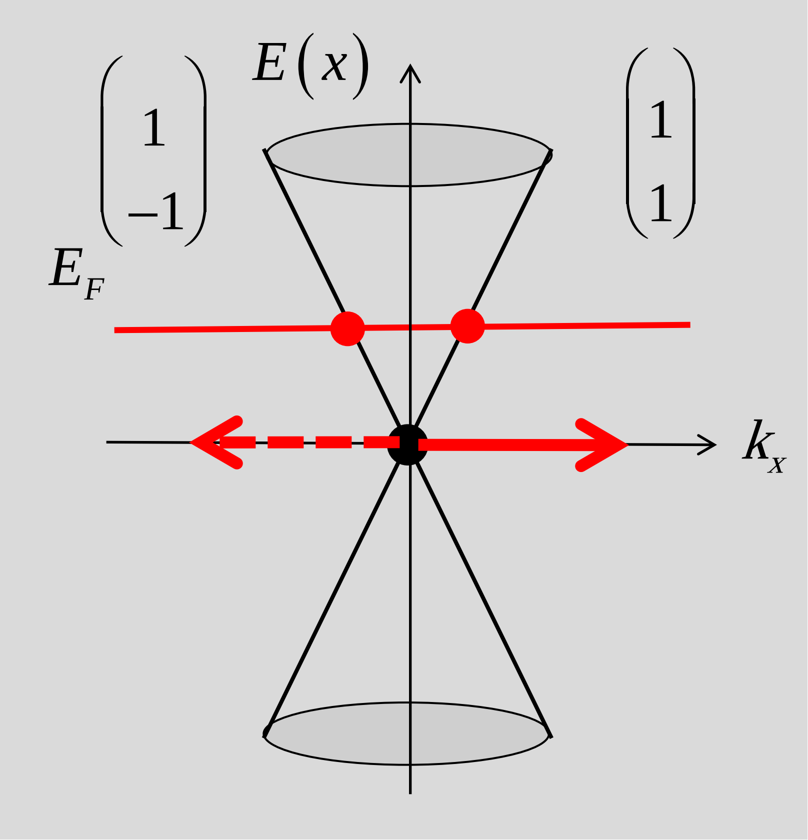
electron wavefunction





$$\psi(x,y) = \frac{1}{\sqrt{A}} e^{i(k_x x + k_y y)}$$

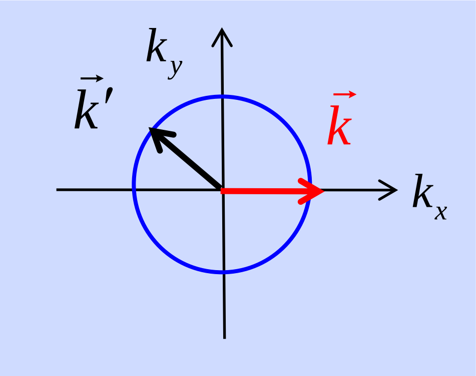
two-component wavefunction



$$\psi(x,y) = \begin{pmatrix} 1 \\ se^{i\theta} \end{pmatrix} e^{i(k_x x + k_y y)}$$

$$s = \mathrm{sgn}(E) \quad \theta = \arctan(k_y/k_x)$$

backscattering is supresed



outline

10.1 Graphene

10.2 Density of states and carrier density

10.3 Number of modes and conductance

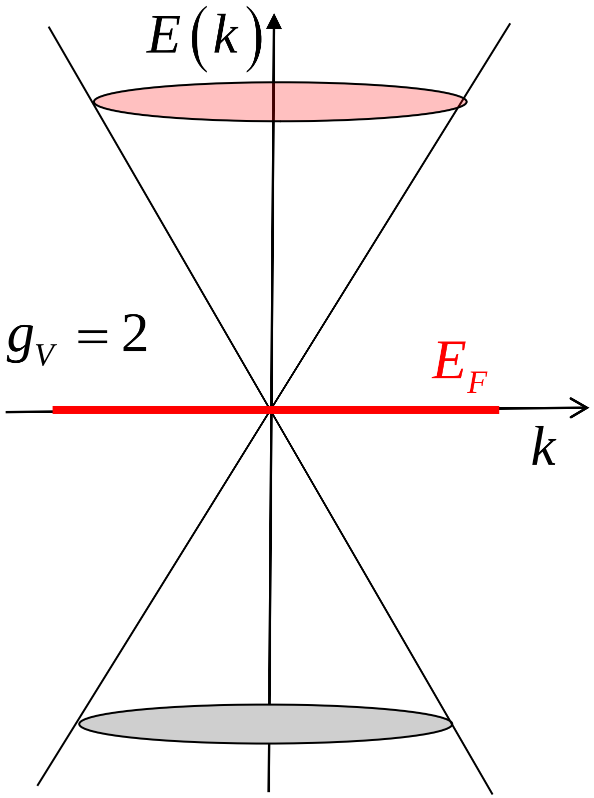
10.4 Scattering

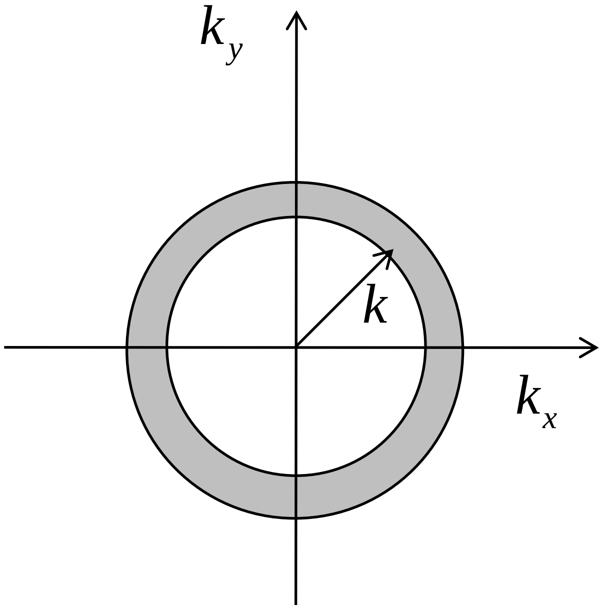
10.5 Conductance vs. carrier density

10.6 Discussion

10.7 Summary

density-of-states



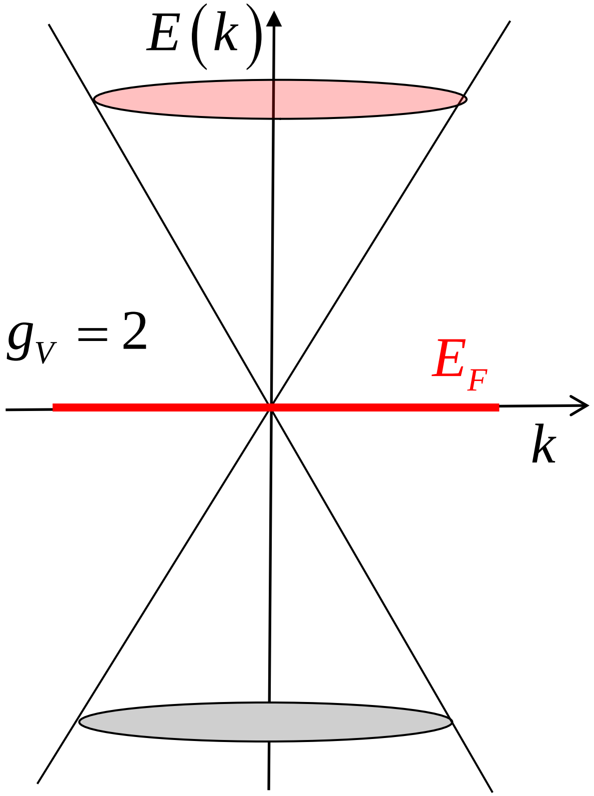


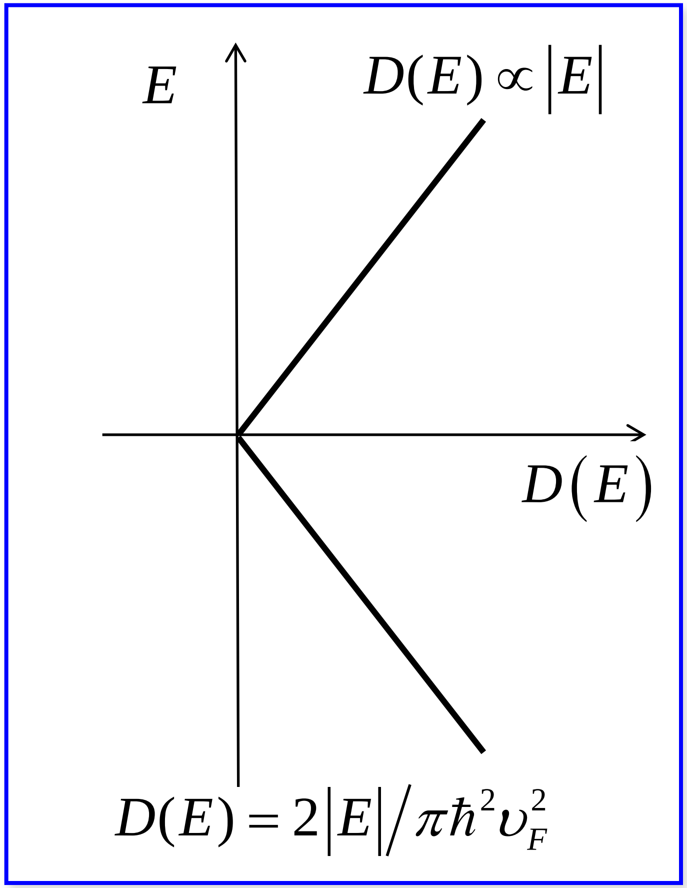
$$N(k)\,dk = \frac{2\pi\, k\,dk}{\left(2\pi/L_x\right)\left(2\pi/L_y\right)} \times 2 \times g_V$$

$$N(k)dk = A g_V \frac{k\,dk}{\pi}$$

$$E(k) = \hbar\upsilon_F k \qquad k\,dk = \frac{E\,dE}{\left(\hbar\upsilon_F\right)^2}$$

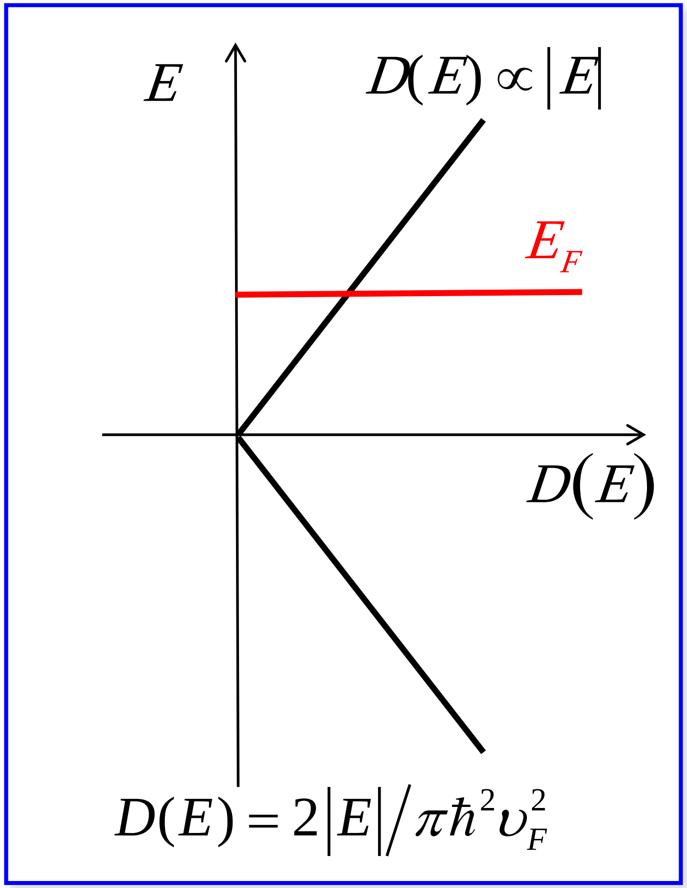
density-of-states





$$N(k)\,dk = Ag_V\frac{k\,dk}{\pi} = Ag_V\frac{E\,dE}{\pi\left(\hbar\upsilon_F\right)^2} = AD\left(E\right)dE$$

carrier density



$$n_S(E_F) = \int_0^\infty D(E) f_0(E)\, dE$$

T_L = 0 K is a good approximation for graphene – even at 300 K.

$$n_S(E_F) = \int_0^{E_F} D(E)\, dE$$

$$n_S(E_F) = \frac{2}{\pi\hbar^2\upsilon_F^2}\int_0^{E_F} E\, dE$$

$$\boxed{n_S(E_F) = \frac{E_F^2}{\pi\hbar^2\upsilon_F^2}}$$

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number of modes

Recall from Lecture 2:

$$M(E) = W\frac{h}{4}\left\langle \upsilon_x^+ \right\rangle D(E)$$

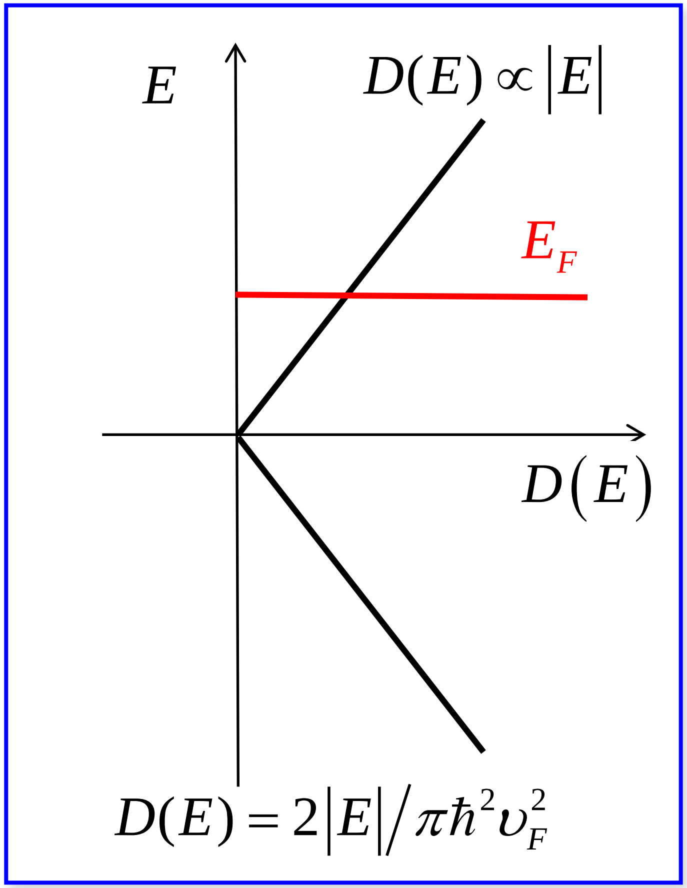
for graphene:

$$D(E) = 2|E| / \pi\hbar^2\upsilon_F^2$$

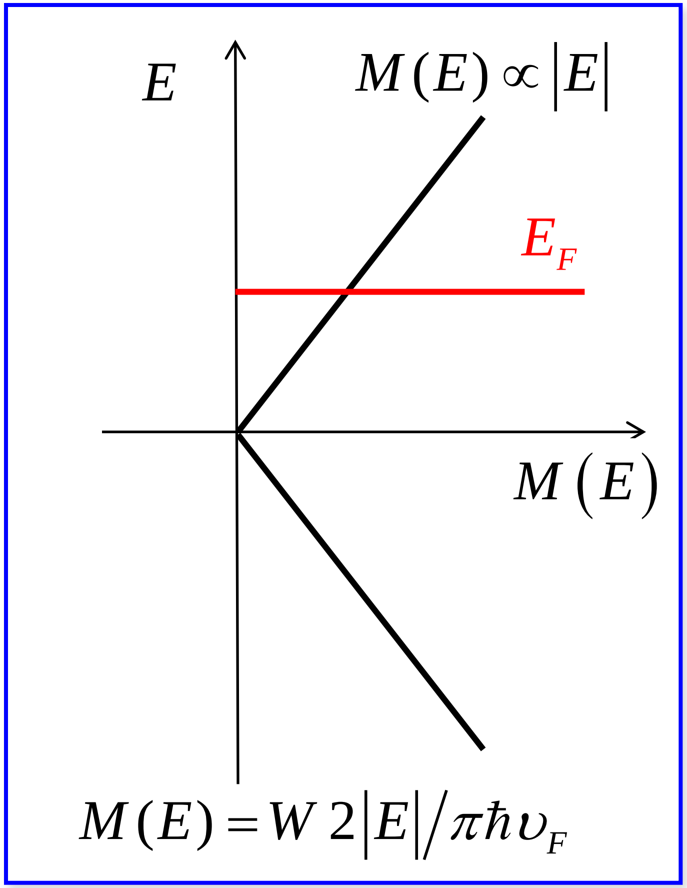
$$\left\langle \upsilon_x^+ \right\rangle = \frac{2}{\pi}\upsilon_F$$

$$M(E) = W\frac{2|E|}{\pi\hbar\upsilon_F}$$

DOS vs. modes

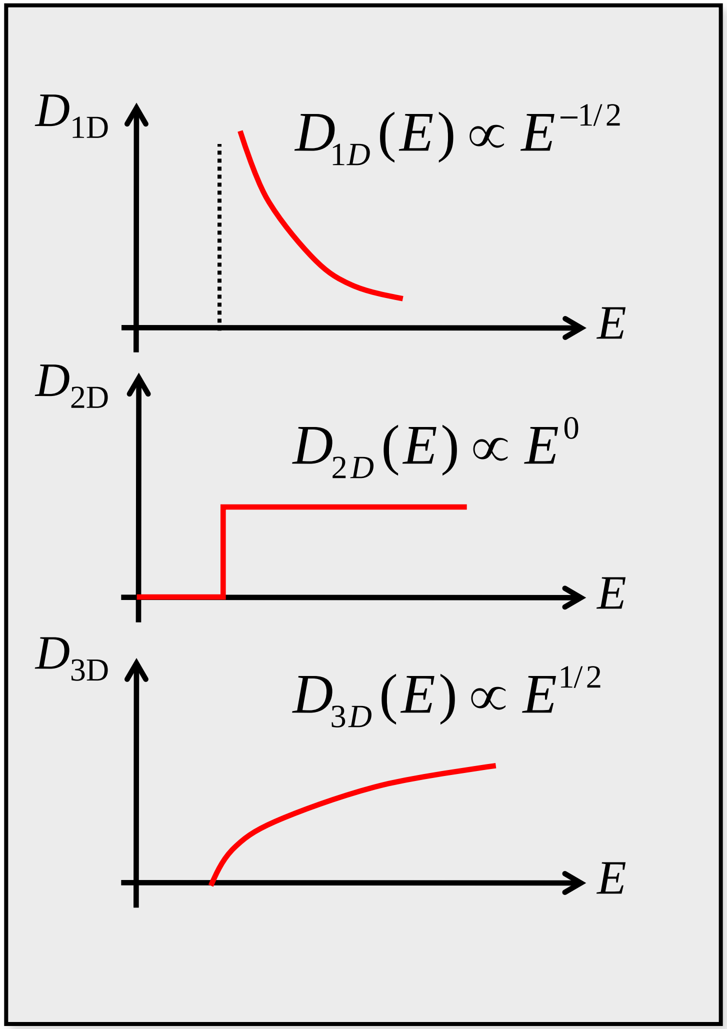


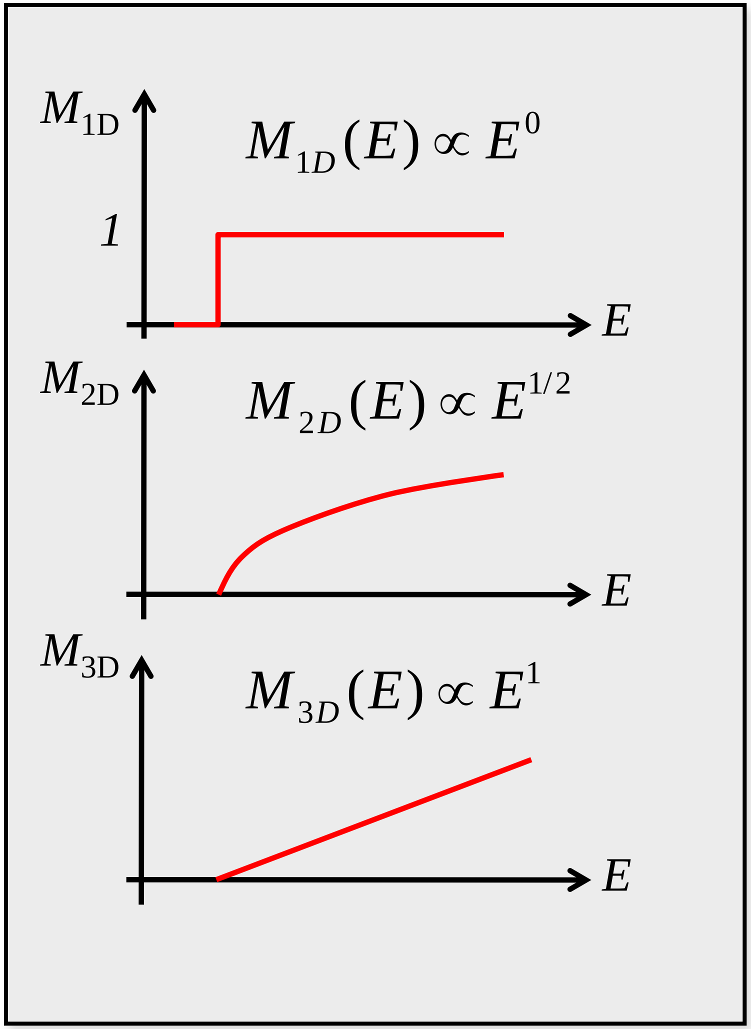
$$D(E) = 2|E| / \pi \hbar^2 \upsilon_F^2$$



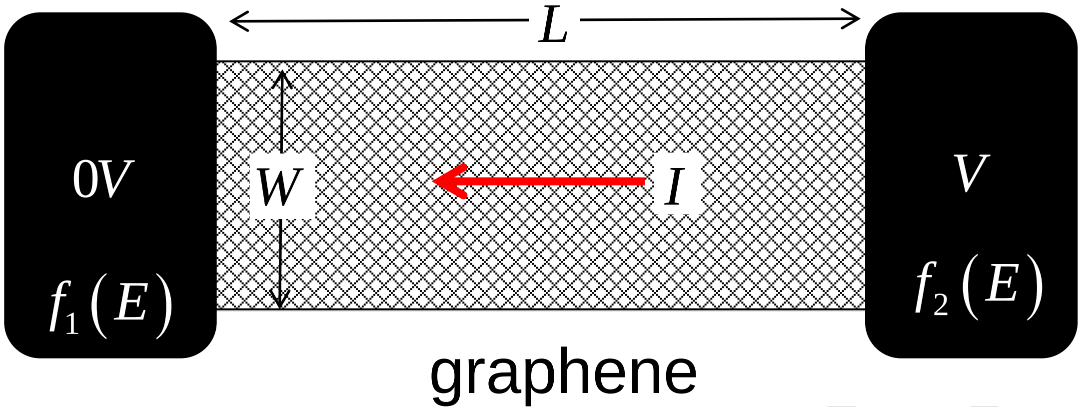
$$M(E) = W\, 2|E| / \pi \hbar \upsilon_F$$

DOS vs. modes (parabolic)





conductance



E_{F1}

$E_{F2} = E_{F1} - qV$

$$I = \frac{2q}{h} \int_{-\infty}^{+\infty} T(E) M(E) \left(f_1 - f_2 \right) dE$$

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

$$\left\{ \begin{array}{l} f_0(E) = 1 \Big/ \left(1 + e^{(E - E_F)/k_B T} \right) \\ T(E) \equiv \lambda(E) \Big/ \left(\lambda(E) + L \right) \\ M(E) = W \, 2 |E| \Big/ \pi \hbar \upsilon_F \end{array} \right.$$

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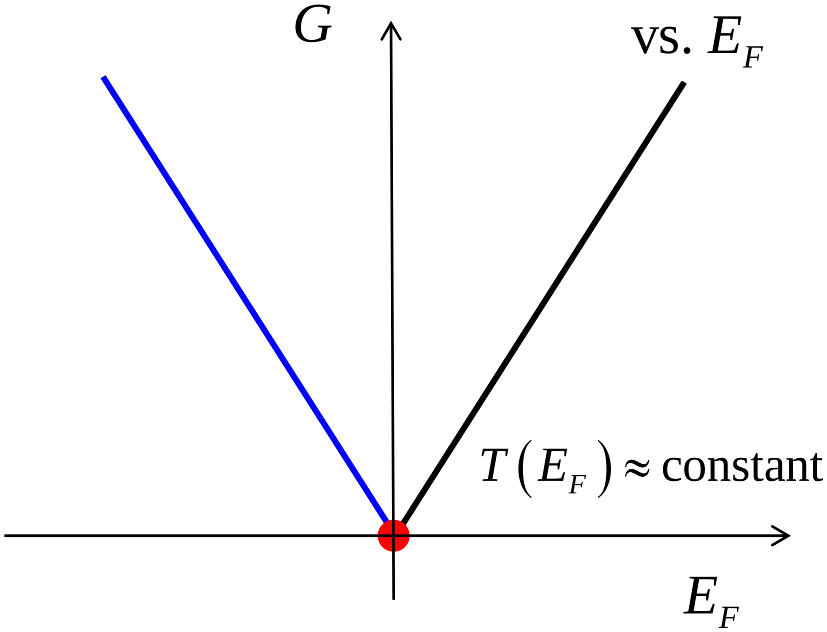
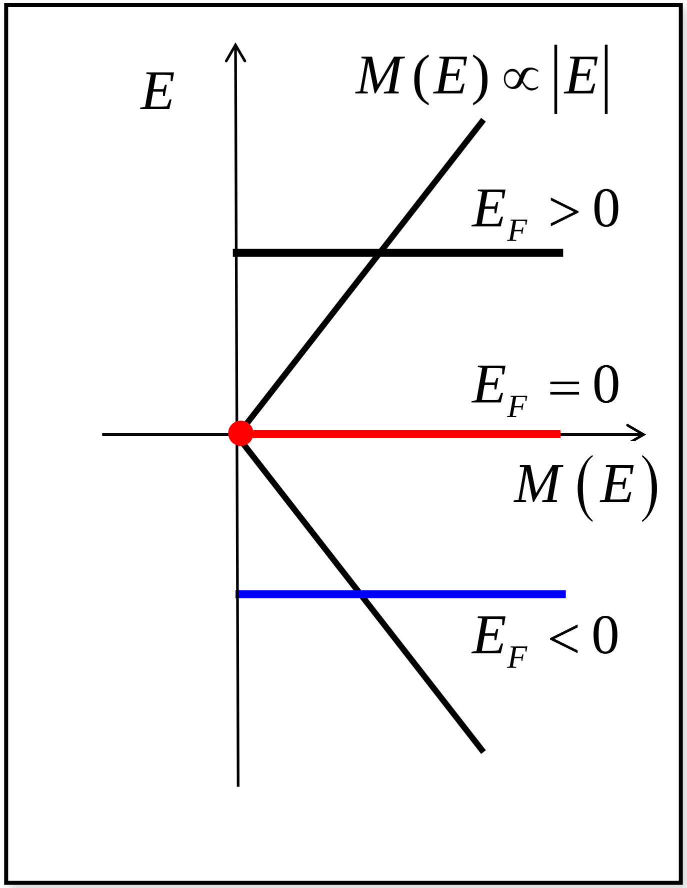
expected results: *G* vs. E_F at T_L = 0K

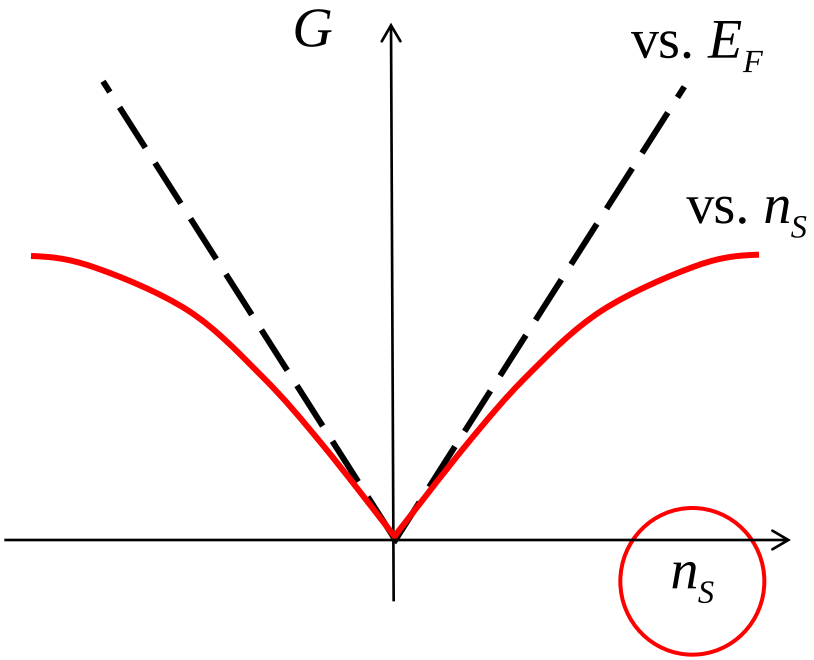


$$-\frac{\partial f_0(E)}{\partial E} = \delta(E - E_F)$$

$$\boxed{G(0\text{K}) = \frac{2q^2}{h} T(E_F) M(E_F)}$$



expected results: *G* vs. n_S at T_L = 0K



$$G = \frac{2q^2}{h} T\left(E_F\right) M\left(E_F\right)$$

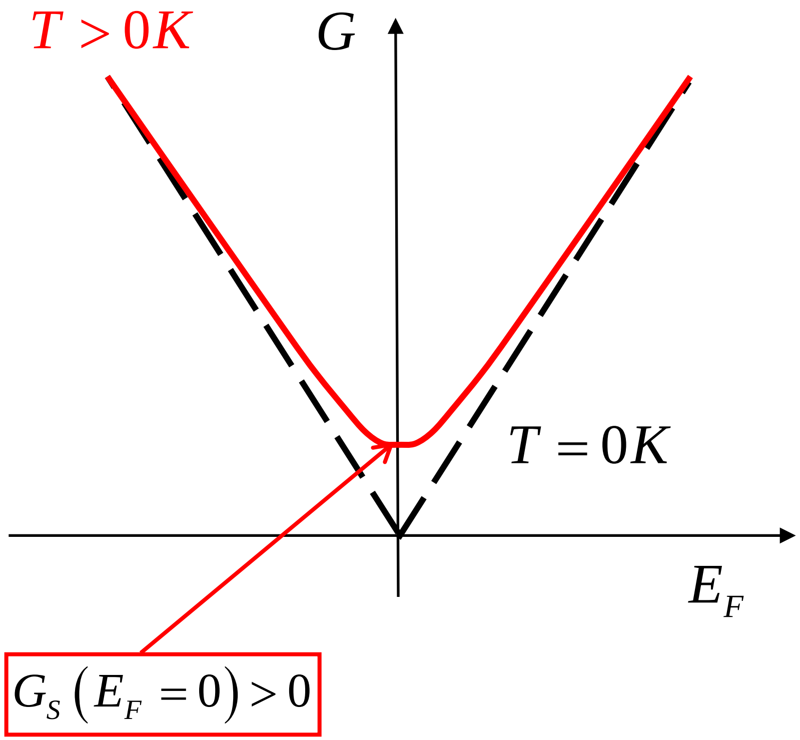
$$n_S\left(E_F\right) = \frac{1}{\pi}\left(\frac{E_F}{\hbar \upsilon_F}\right)^2 \propto E_F^2$$

$$M\left(E_F\right) \propto E_F \propto \sqrt{n_S}$$

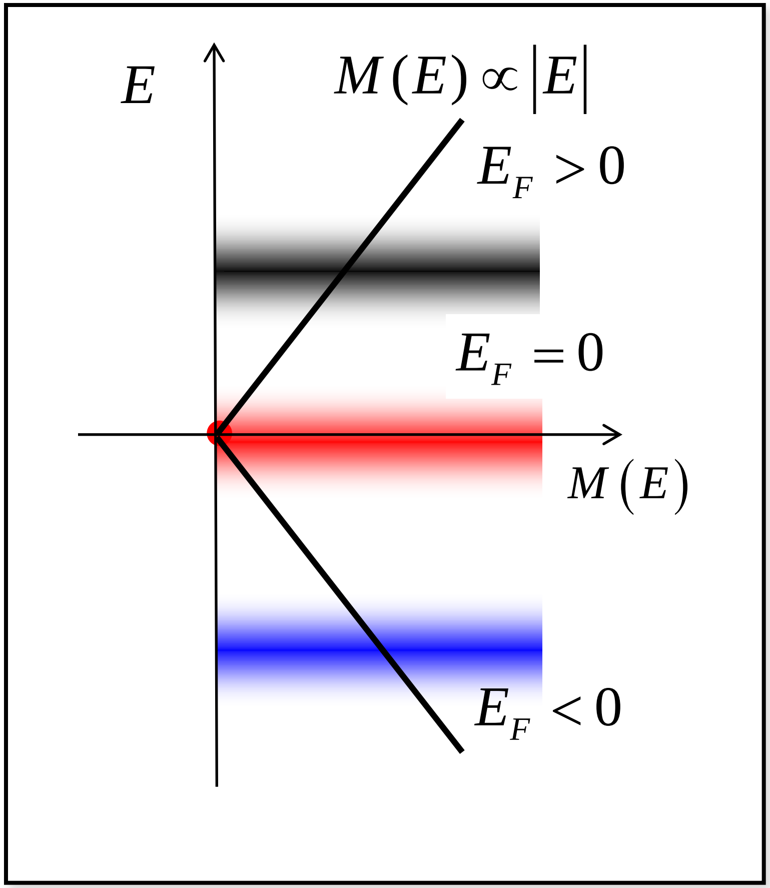
$$G \propto \sqrt{n_S}$$

$$\left(T\left(E_F\right) \approx \text{constant}\right)$$

expected results: $T_L > 0\text{K}$



$G_S(E_F = 0) > 0$



$$G(T_L > 0K) = \frac{2q^2}{h}\langle T(E_F)M(E_F)\rangle$$

some key equations (T_L = 0K)

$$G\left(0K\right)=\frac{2q^2}{h}T(E_F)M(E_F)$$

$$M(E_F)=W\,2E_F/\pi\hbar\upsilon_F$$

$$T\left(E_F\right)=\lambda\left(E_F\right)\big/\left(\lambda\left(E_F\right)+L\right)$$

$$G\left(0K\right)=\frac{2q^2}{h}\frac{\lambda(E_F)}{\lambda(E_F)+L}W\frac{2E_F}{\pi\hbar\upsilon_F}$$

$$G=\sigma_S\frac{W}{L}$$

$$\sigma_S\left(0\mathrm{K}\right)=\frac{2q^2}{h}\lambda_{app}\left(\frac{2E_F}{\pi\hbar\upsilon_F}\right)$$

Describes the conductance of the conduction (E > 0) or valence (E < 0) bands.

(For T_L > 0, the total conductance is the sum of the two.)

σ_s is the “sheet conductance.”

$$\frac{1}{\lambda_{app}}=\frac{1}{\lambda\left(E_F\right)}+\frac{1}{L}$$

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conductance and scattering

$$G(0\mathrm{K}) = \frac{2q^2}{h}\left(\frac{\lambda(E_F)}{\lambda(E_F)+L}\right)\left(W\frac{2E_F}{\pi\hbar\upsilon_F}\right)$$

λ(*E*) is the mean-free-path for backscattering, which is determined by the dominant scattering processes.

$$\lambda(E) = \frac{\pi}{2}\upsilon_F \tau_m(E)$$

scattering

For many scattering mechanisms (e.g. acoustic phonon, point defect), the scattering rate is proportional to the density of final states:

$$\frac{1}{\tau(E)} \propto D(E) \propto E \qquad \tau(E) \propto E^{-1}$$

The energy-dependent mean-free-path is:

$$\lambda(E) \propto 1/E$$

What does this type of scattering do to the conductance?

effect of short range / ADP scattering

Assume T_L = 0 K and diffusive transport (just to keep the math simple)

$$\sigma_S = \frac{2q^2}{h}\lambda(E_F)\left(\frac{2E_F}{\pi\hbar\upsilon_F}\right) \qquad \lambda(E_F) \propto 1/E_F \qquad \sigma_S = \text{constant!}$$

For short range or ADP scattering, σ_S is constant.

$$\sigma_S = n_S q \mu_n \Rightarrow \mu_n \propto \frac{1}{n_S}$$

N.H. Shon and T. Ando, *J. Phys. Soc*. Japan, **67**, 2421, 1998.

maximum conductivity of graphene

$$\sigma_S = \frac{2q^2}{h}\lambda\left(E_F\right)\left(\frac{2E_F}{\pi\hbar\upsilon_F}\right)$$

$$\tau_m\left(E\right) = \frac{4\mathrm{h}^3\rho_m\upsilon_F^2\upsilon_S^2}{\mathrm{D}_A^2 k_B T_L}\left(\frac{1}{E}\right) \qquad \lambda\left(E\right) = \frac{2\pi\hbar^3\rho_m\upsilon_F^3\upsilon_S^2}{\mathrm{D}_A^2 k_B T_L}\left(\frac{1}{E}\right)$$

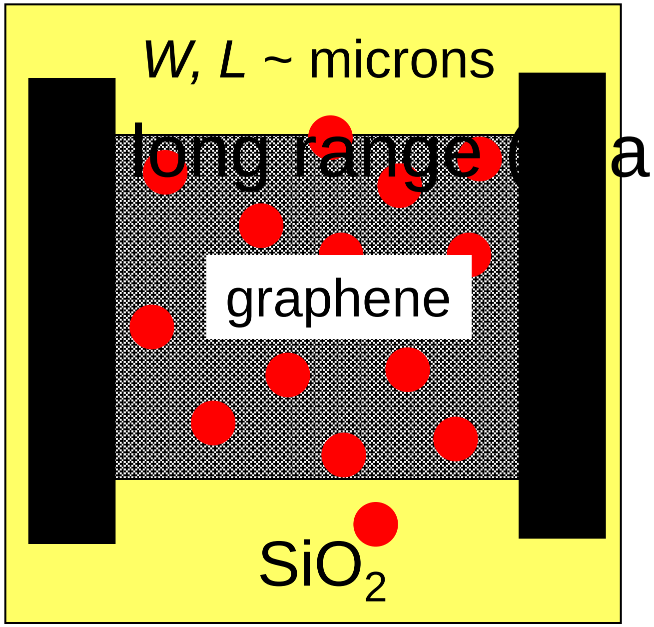
(ADP scattering)

$$\sigma_S = \frac{4q^2\mathrm{h}\rho_m\upsilon_F^2\upsilon_S^2}{\pi D_A^2 k_B T_L}$$

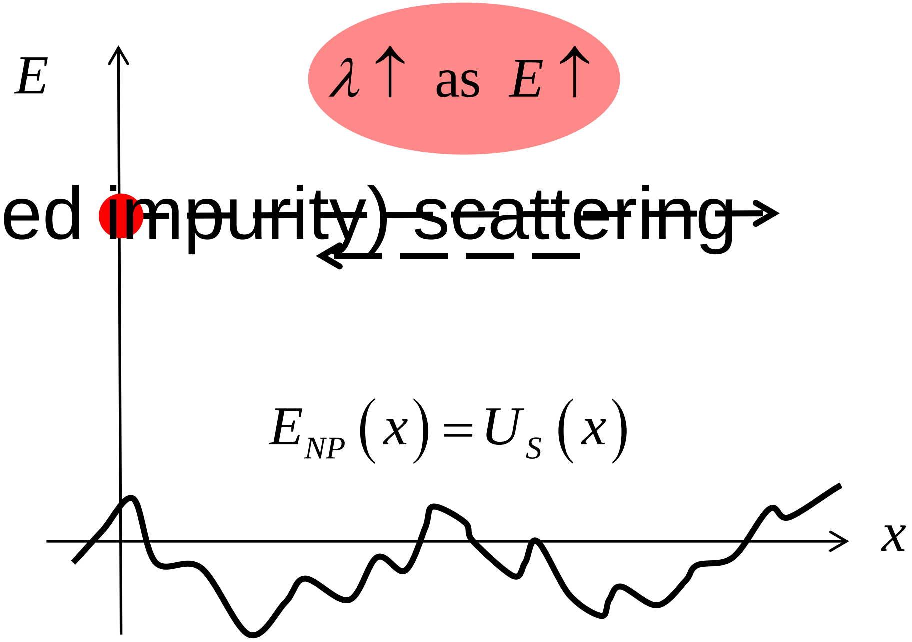
$$\left\{\begin{array}{l} \upsilon_S \approx 2.1\times 10^4\ \ \mathrm{m/s} \\ \rho_m \approx 7.6\times 10^{-7}\ \ \mathrm{kg/m^2} \\ D_A \approx 18\,\mathrm{eV} \end{array}\right\}$$

$$\rho_S \approx 30\ \Omega\,/\mathrm{W}$$

long range (charged impurity) scattering



Top view



long range (charged impurity) scattering

For screened or unscreened charged impurity scattering, the mfp is **proportional** to energy.

Random charges introduce random fluctuations in $E(k)$, which act a scattering centers.

High energy electrons don’t “see” these fluctuations and are not scattered as strongly.

effect of charged impurity scattering

Assume T_L = 0 K and diffusive transport (just to keep the math simple)

$$\sigma_S = \frac{2q^2}{h}\lambda(E_F)\left(\frac{2E_F}{\pi\hbar\upsilon_F}\right) \qquad \lambda(E_F) \propto E_F$$

$$\sigma_S \propto n_S \qquad (\mu_n \quad \text{constant})$$

For charged impurity scattering, σ_S vs. n_S is linear.

T. Ando, *J. Phys. Soc. Japan*, **75**, 074716, 2006

N.M.R. Peres, J.M.B. Lopes dos Santos, and T. Stauber, *Phys. Rev. B*, **76**, 073412, 2007.

outline

Acknowledgement: The calculations done in this section were performed by Dionisis Berbedes.

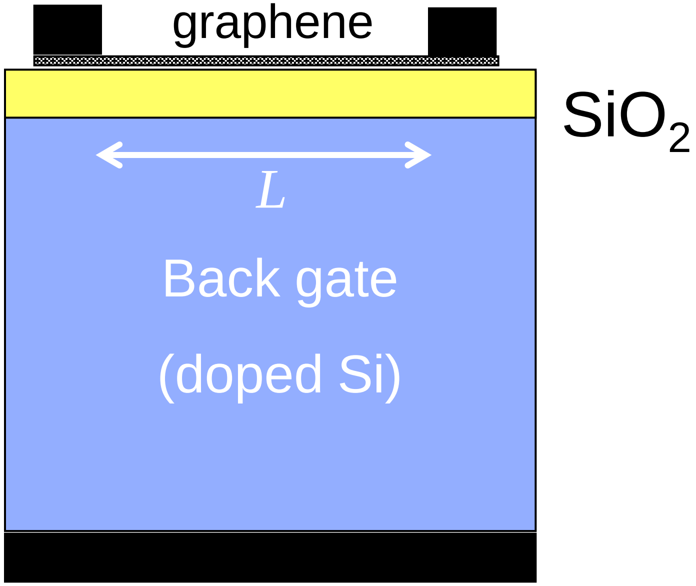
gate-modulated conductance in graphene

1) The location of the Fermi level (or equivalently the carrier density) is experimentally controlled by a “gate.”

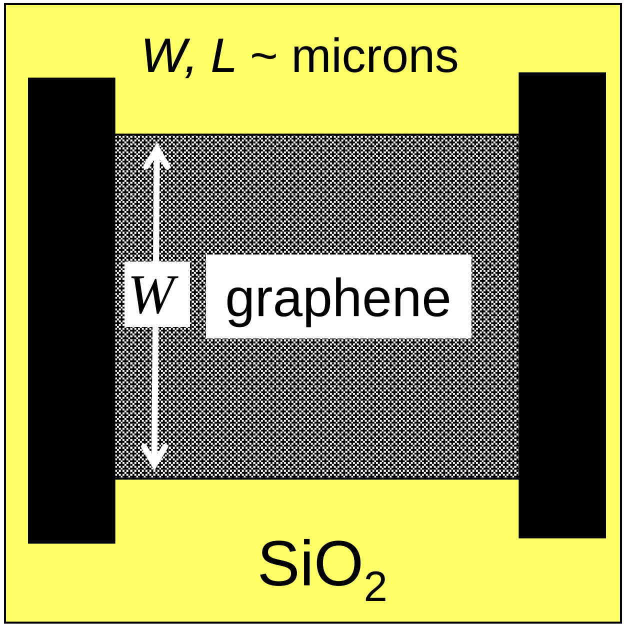
2) In a typical experiments, a layer of graphene is placed on a layer of SiO_2, which is on a doped silicon substrate. By changing the potential of the Si substrate (the “back gate”), the potential in the graphene can be modulated to vary E_F and, therefore, n_S.

experimental structure (2-probe)

(4-probe techniques are used to eliminate series resistance and for Hall effect measurements.)



Side

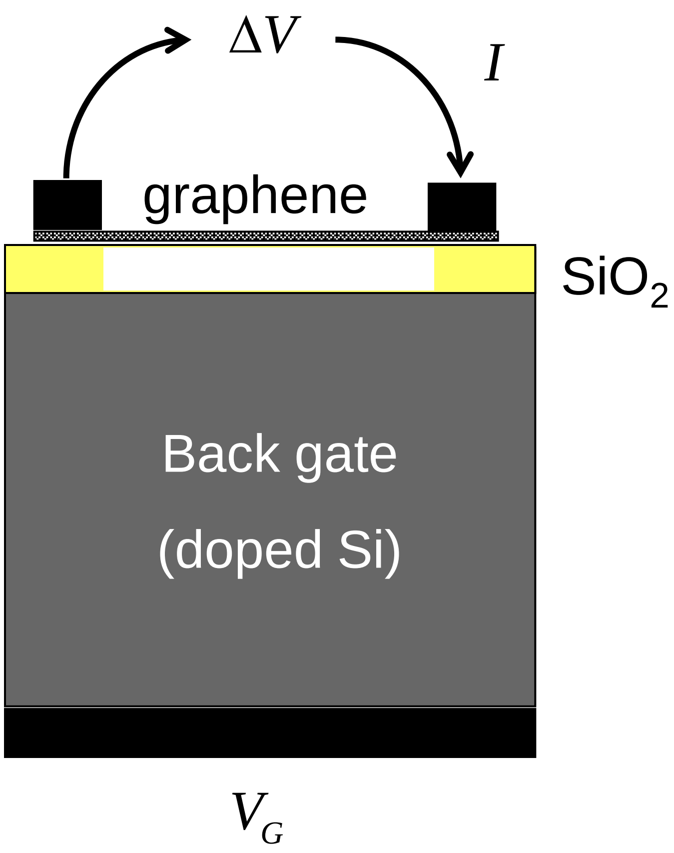


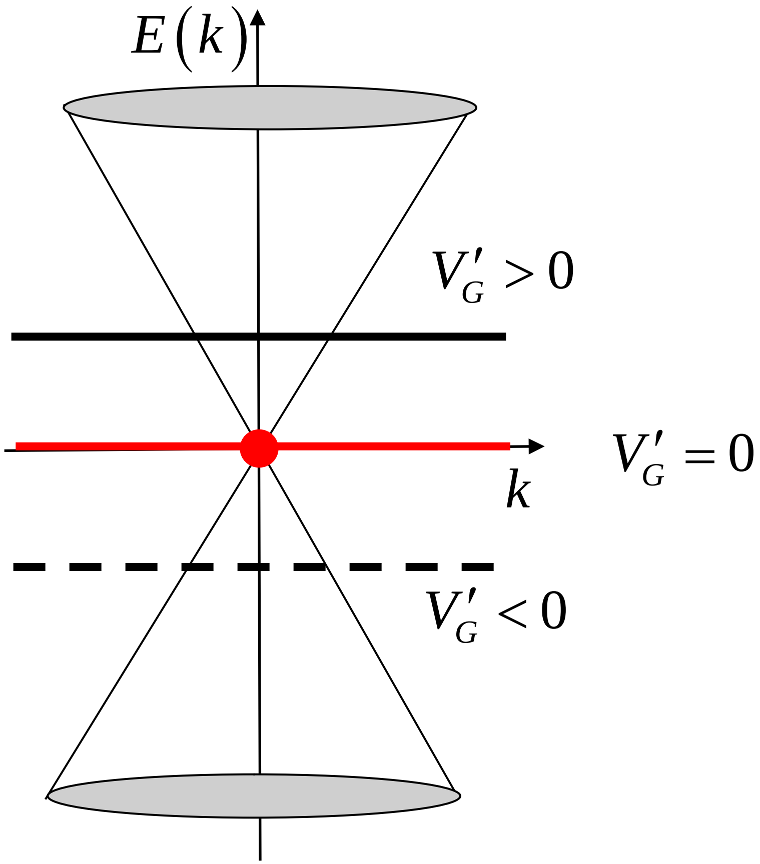
Top view

Typically, Cr/Au or Ti/Au are used for the metal contacts.

The thickness of SiO$_2$ is typically 300nm or 90nm, which makes it possible to see a single layer of graphene.

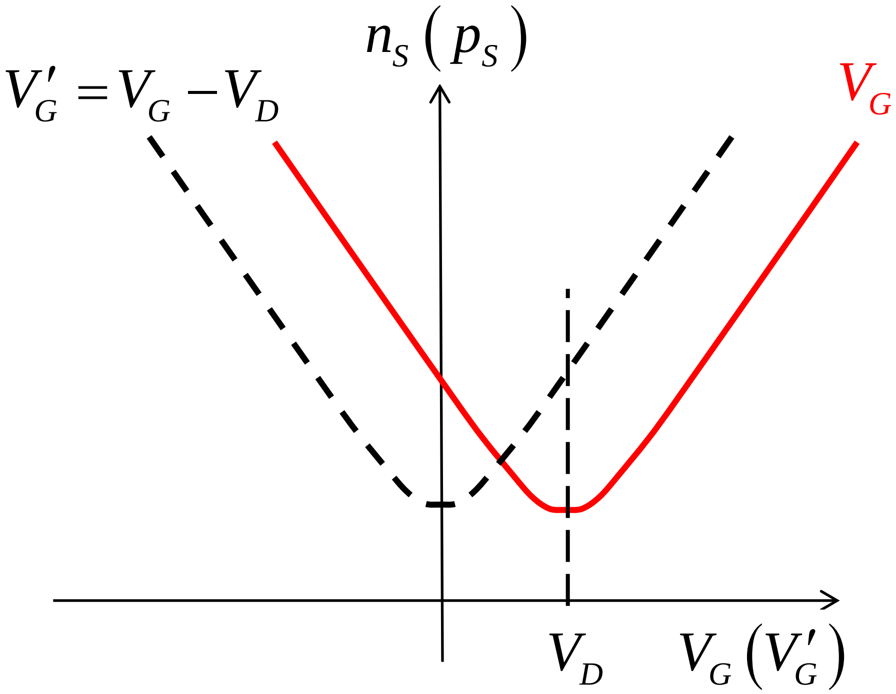
using a gate voltage to change the Dirac point (or E_F)





$$V_G' = V_G - V_D$$

gate voltage - carrier density relation



If the oxide is not too thin (so that the quantum capacitance of the graphene is not important), then

$$qn_S = C_{ins} V_G'$$

$$C_{ins} = \frac{\varepsilon_{ins}}{t_{ins}}$$

sheet conductance vs. V_G

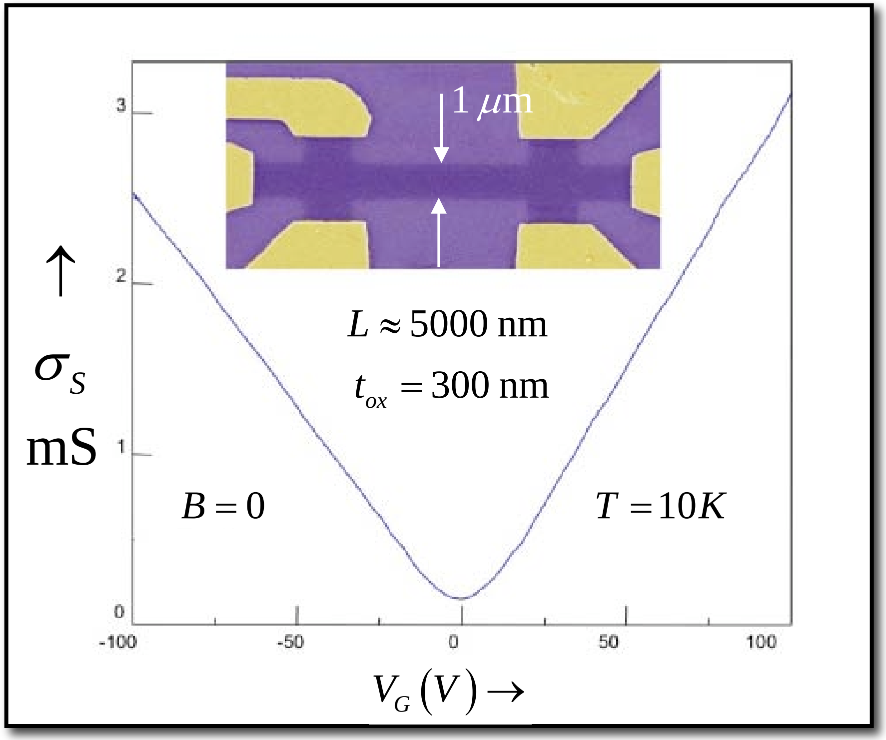


Fig. 30 in A. H. Castro, et al.,“The electronic properties of graphene,” Rev. of Mod. Phys., **81**, 109, 2009.

$$G = \sigma_S W/L$$

$$\sigma_S(E_F) \approx \frac{2q^2}{h} \lambda_{app}(E_F) \left(\frac{2E_F}{\pi \hbar \upsilon_F} \right)$$

$$n_S = C_{ox} V_G \approx \frac{1}{\pi} \left(\frac{E_F}{\hbar \upsilon_F} \right)^2$$

$$\lambda_{app}(E_F) = \frac{\sigma_S / \left(2q^2/h \right)}{2\sqrt{n_S/\pi}}$$

$$\left(T_L = 0 \text{ K} \right)$$

mean-free-path ($V_G = 100\text{V}$)

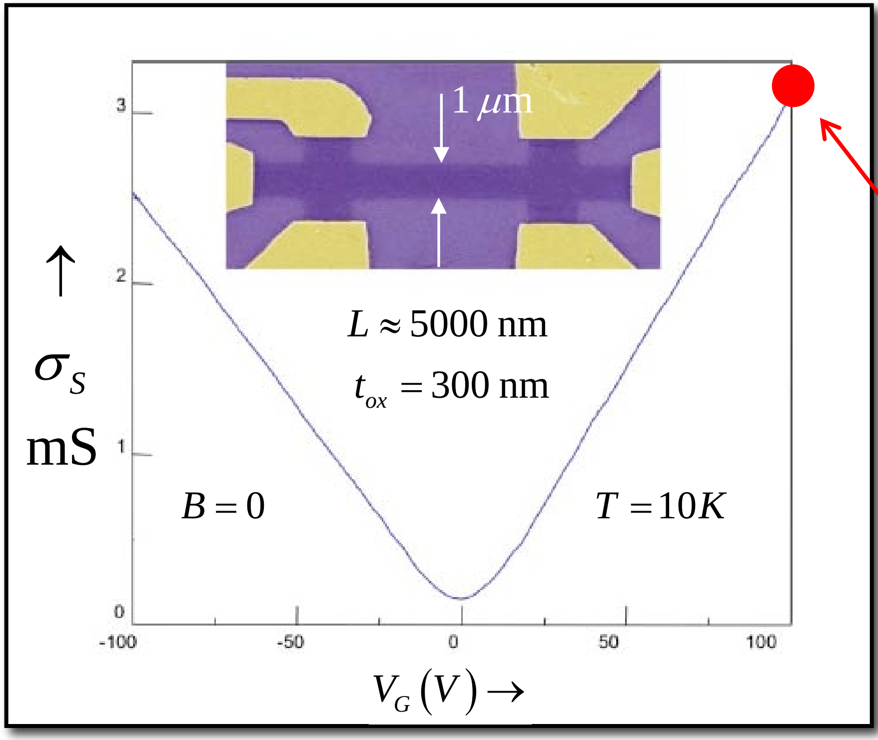


Fig. 30 in A. H. Castro, et al.,“The electronic properties of graphene,” Rev. of Mod. Phys., **81**, 109, 2009.

$$\sigma_S \approx 3.0\ \text{mS}$$

$$n_S \approx 7.1\times10^{12}\ \text{cm}^{-2}$$

$$E_F \approx 0.3\ \text{eV}$$

$$\lambda_{app}(0.3\ \text{eV}) \approx 130\ \text{nm}$$

$$\lambda(0.3\ \text{eV}) << L$$

mean-free-path (V_G = 50V)

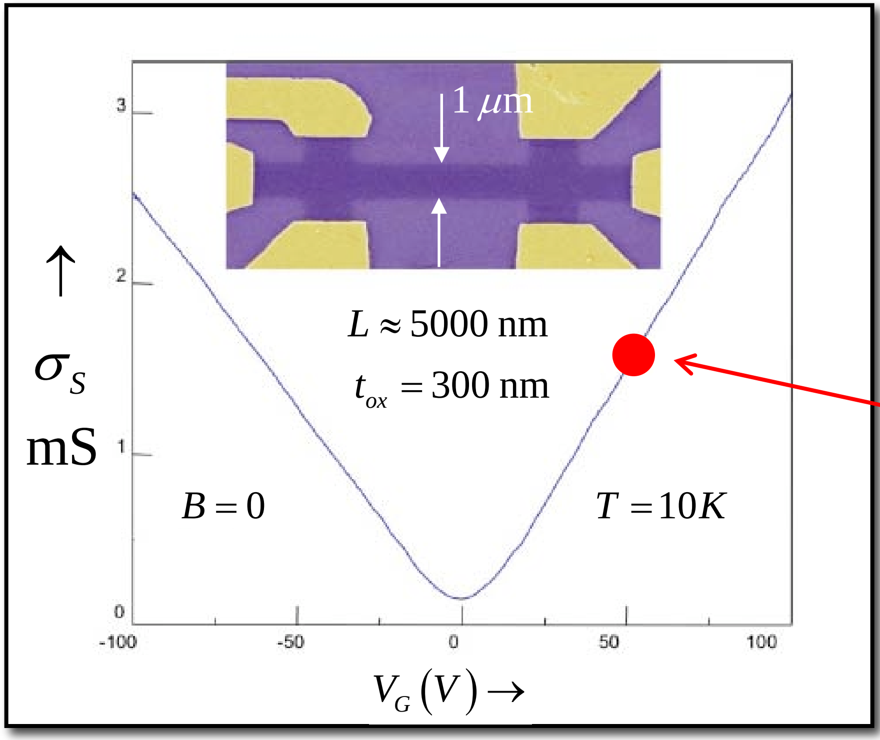


Fig. 30 in A. H. Castro, et al.,“The electronic properties of graphene,” Rev. of Mod. Phys., **81**, 109, 2009.

$$\sigma_S \approx 1.5 \text{ mS}$$

$$n_S \approx 3.6 \times 10^{12} \text{ cm}^{-2}$$

$$E_F \approx 0.2 \text{ eV}$$

$$\lambda_{app}\left(0.2 \text{ eV}\right) \approx 90 \text{ nm}$$

$$\frac{\lambda\left(0.2 \text{ eV}\right)}{\lambda\left(0.3 \text{ eV}\right)} \approx 0.69$$

$$\frac{0.2 \text{ eV}}{0.3 \text{ eV}} \approx 0.67$$

$$\lambda\left(E_F\right) \propto E_F$$

mobility

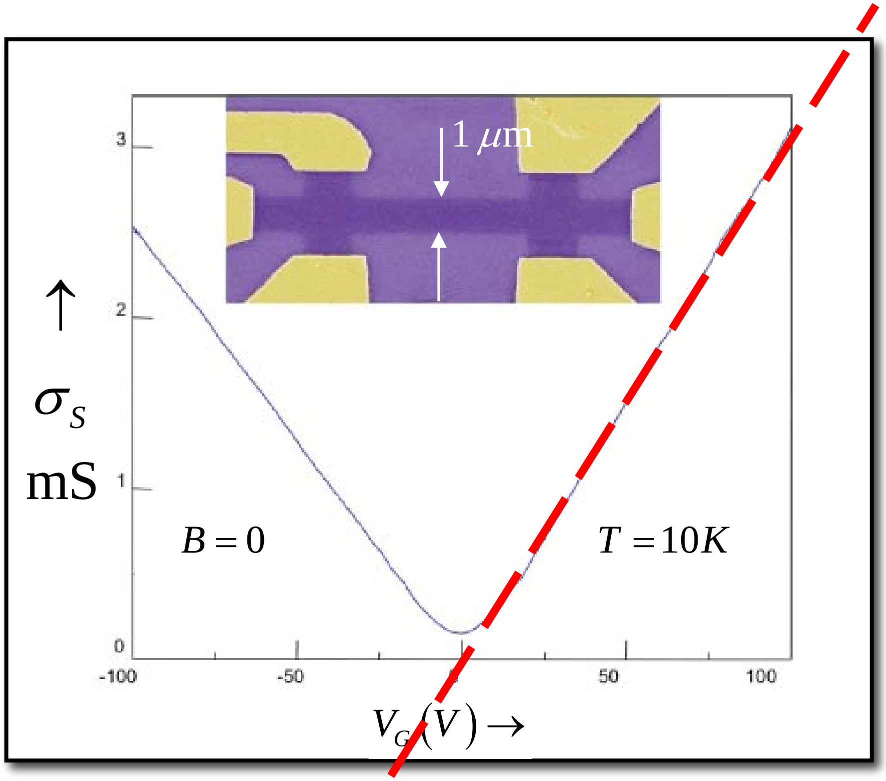


Fig. 30 in A. H. Castro, et al.,“The electronic properties of graphene,” Rev. of Mod. Phys., **81**, 109, 2009.

Since, $\sigma_S \sim n_S$, we can write:

$$\sigma_S \equiv n_S q \mu_n$$

and deduce a mobility:

$$\mu_n \approx 12{,}500 \text{ cm}^2/\text{V-sec}$$

Mobility is constant, but mean-free-path depends on the Fermi energy (or n_S).

electron-hole puddles

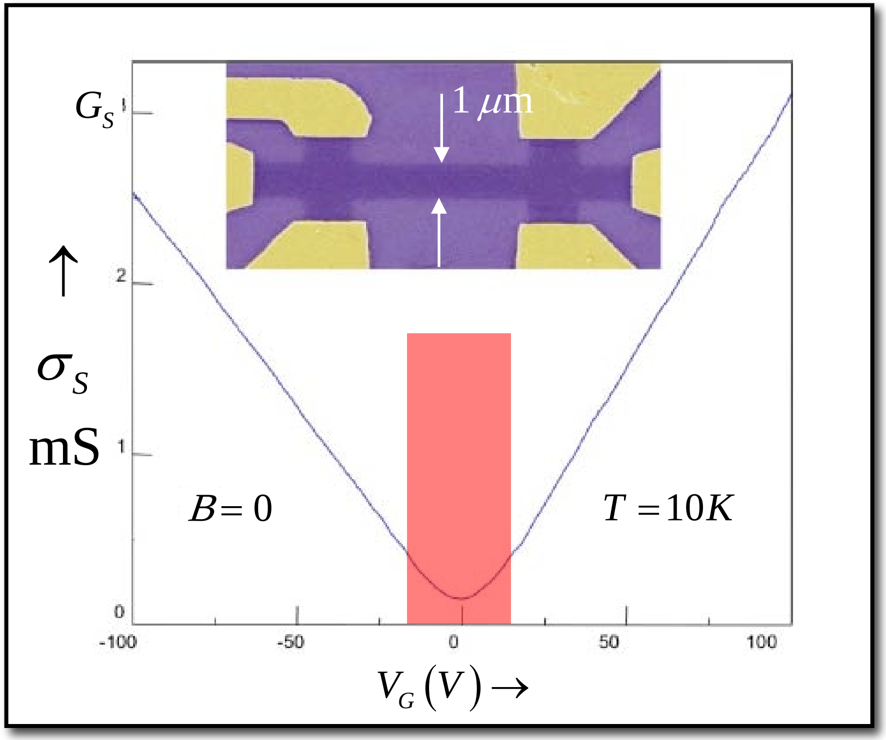
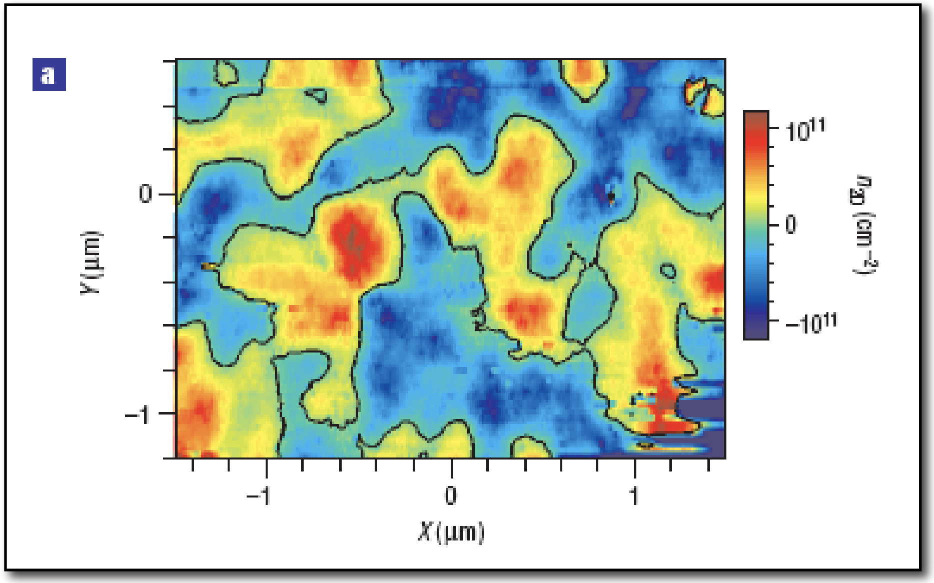
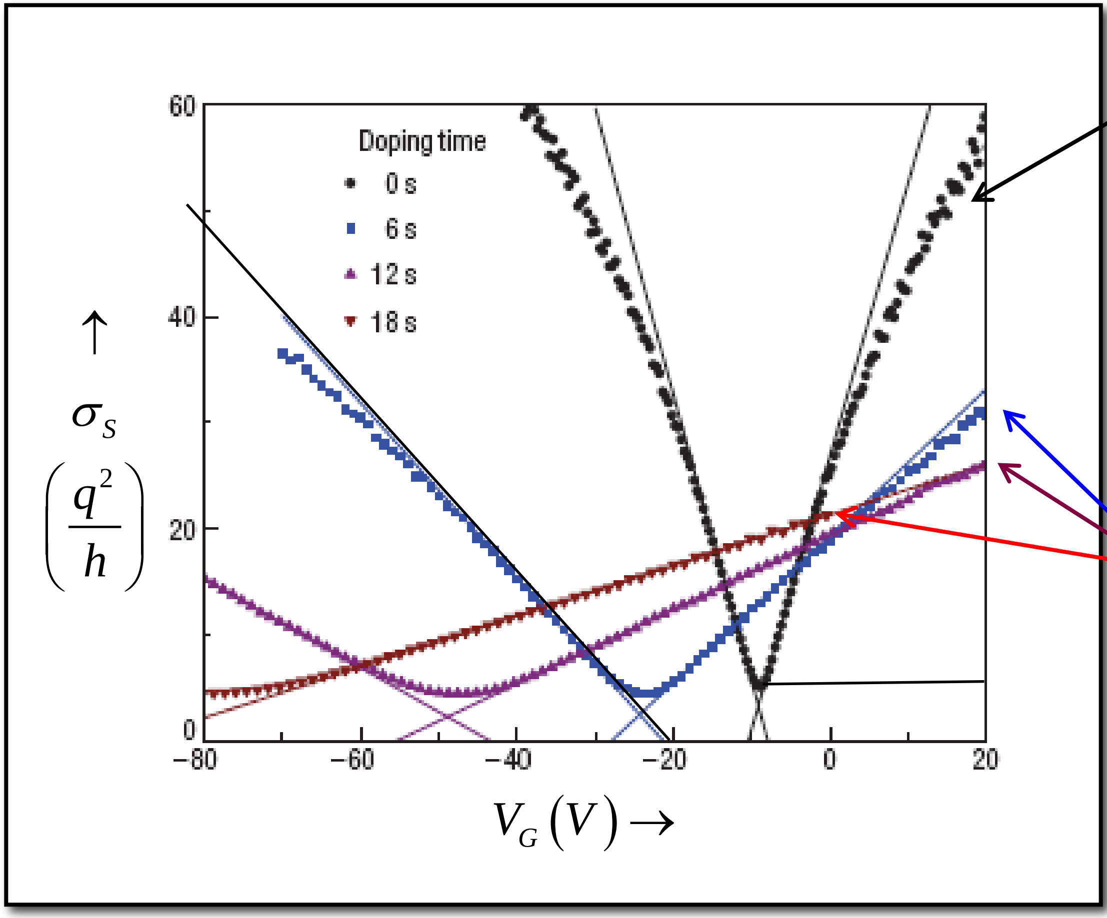


Fig. 30 in A. H. Castro, et al.,“The electronic properties of graphene,” Rev. of Mod. Phys., **81**, 109, 2009.



J. Martin, et al, “Observation of electron–hole puddles in graphene using a scanning single-electron transistor,” Nature Phys., **4**, 144, 2008

effect of potassium doping

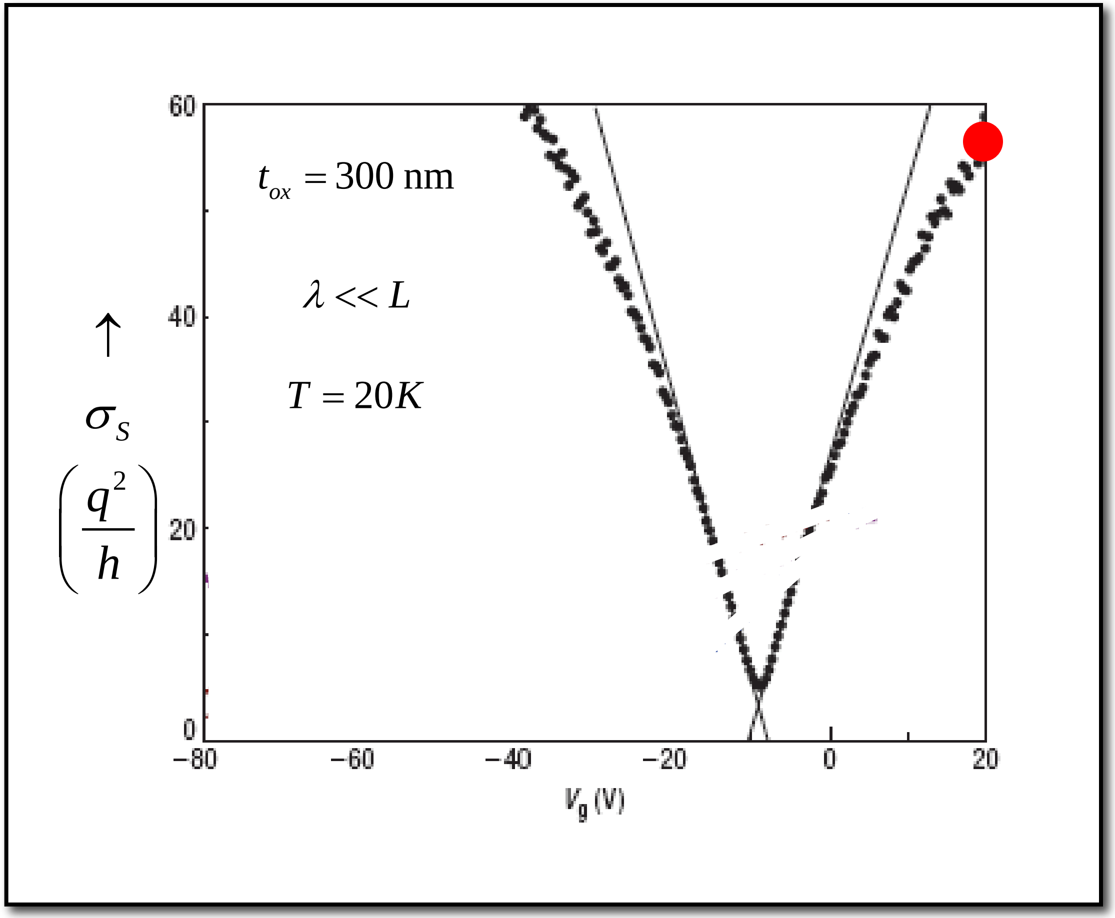


For nominally undoped samples, σ_S vs. n_S is non-linear.

As doping increases, σ_S vs. n_S becomes more linear, mobility decreases, and the NP shifts to the left.

J.-H. Chen, C. Jang, S. Adam, M. S. Fuhrer, E. D. Williams,and M. Ishigami, “Charged-impurity scattering in graphene,” *Nature Phys.*, **4**, 377-381, 2008.

nominally undoped sample: is it ballistic?



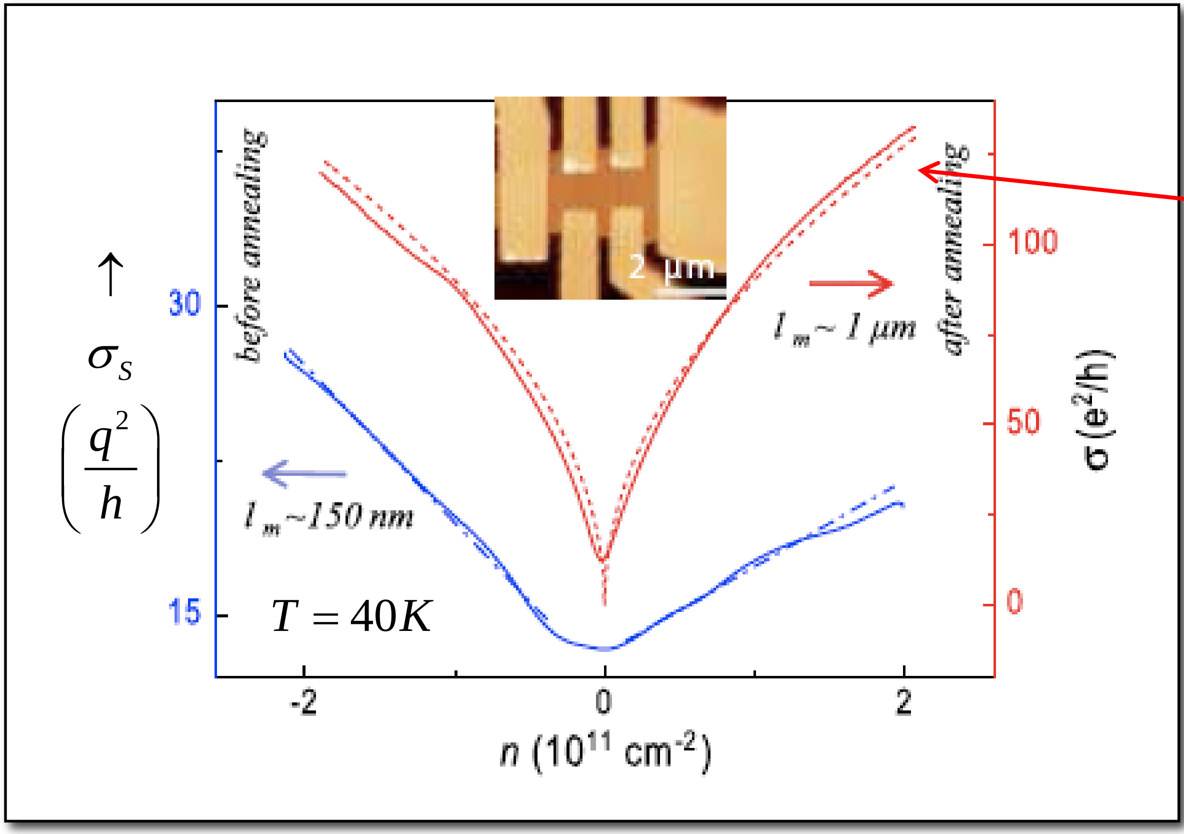
$$\frac{1}{\lambda_{app}} = \frac{1}{\lambda} + \frac{1}{L}$$

$$\lambda_{app} = \frac{\sigma_S / \left(2q^2/h\right)}{2\sqrt{n_S/\pi}} \approx 164 \text{ nm}$$

$$\lambda << L$$

J.-H. Chen, C. Jang, S. Adam, M. S. Fuhrer, E. D. Williams,and M. Ishigami, “Charged-impurity scattering in graphene,” *Nature Phys*., **4**, 377-381, 2008.

unannealed vs. annealed suspended graphene



$$\sigma_S \propto \sqrt{n_S}$$

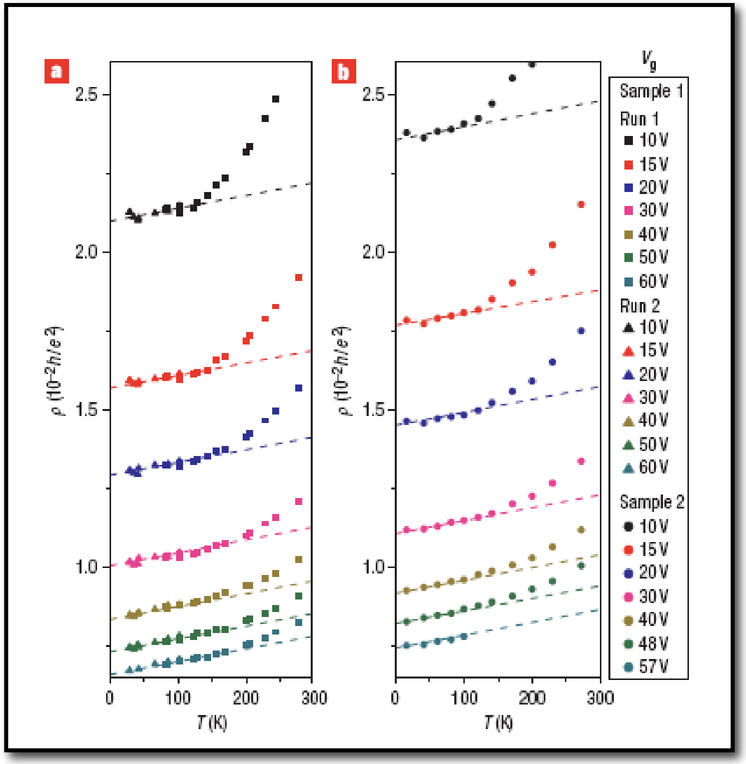
$$\lambda_{app} \approx 1300 \text{ nm}$$

expected from ballistic theory

K. I. Bolotin, K. J. Sikes, J. Hone, H. L. Stormer, and P. Kim, “Temperature dependent transport in suspended graphene,” 2008

temperature dependence

Away from the conductance minimum, the conductance decreases as T_L increases (or resistivity increases as temperature increases).



$$T_L < 100K: \quad R_S \propto T_L$$

(acoustic phonon scattering - intrinsic)

$$T_L > 100K: \quad R_S \propto e^{\hbar\omega_0/k_B T_L}$$

(optical phonons in graphene or surface phonons at SiO_2 substrate)

J.-H. Chen, J. Chuan, X. Shudong, M. Ishigami, and M.S. Fuhrer, "Intrinsic and extrinsic performance limits of graphene devices on SiO_2," Nature Nanotechnology, **3**, pp. 206-209, 2008.

phonons and temperature dependence

$$R_S = \frac{1}{G_S} \propto \frac{1}{\lambda} \propto \frac{1}{\tau} \propto n_0$$

$$n_0 = \frac{1}{e^{\hbar\omega(\beta)/k_B T_L} - 1}$$

acoustic phonons:

$$\hbar\omega < k_B T_L$$

$$N_\beta \approx \frac{k_B T_L}{\hbar\omega}$$

$$R_S \propto T_L$$

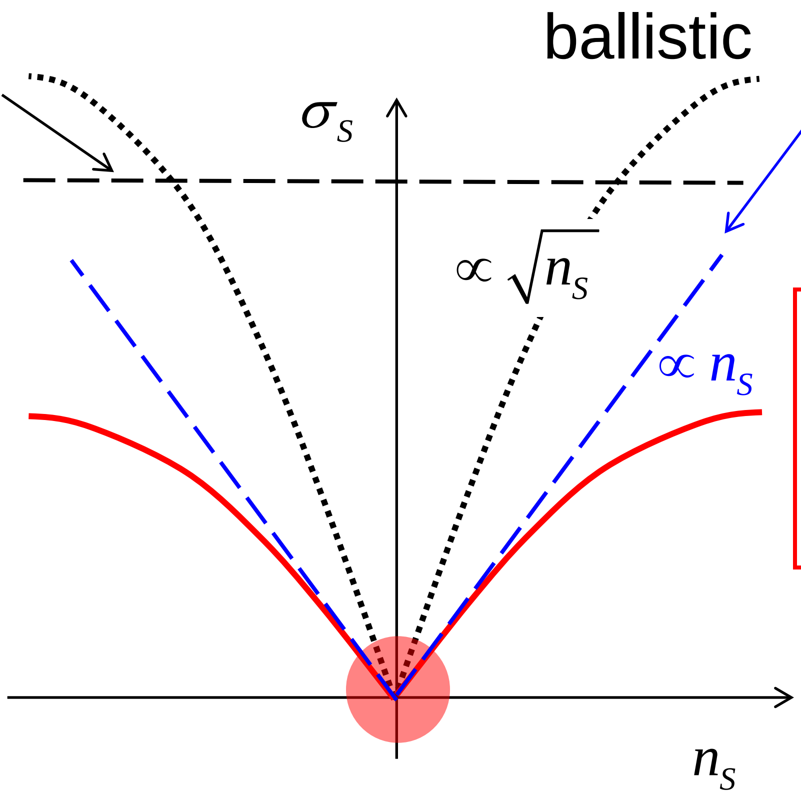
optical phonons:

$$\hbar\omega_0 \approx k_B T_L$$

$$n_0 = \frac{1}{e^{\hbar\omega_0/k_B T_L} - 1}$$

$$R_S \propto \frac{1}{e^{\hbar\omega_0/k_B T_L} - 1}$$

general picture of σ_S vs. n_S (diffusive)



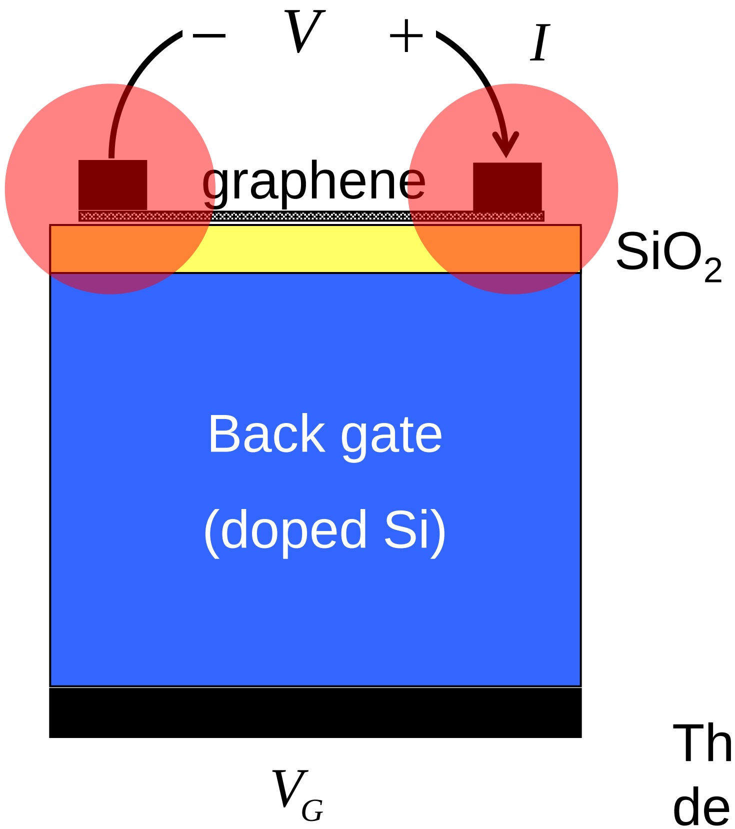
Short range or acoustic phonon scattering.

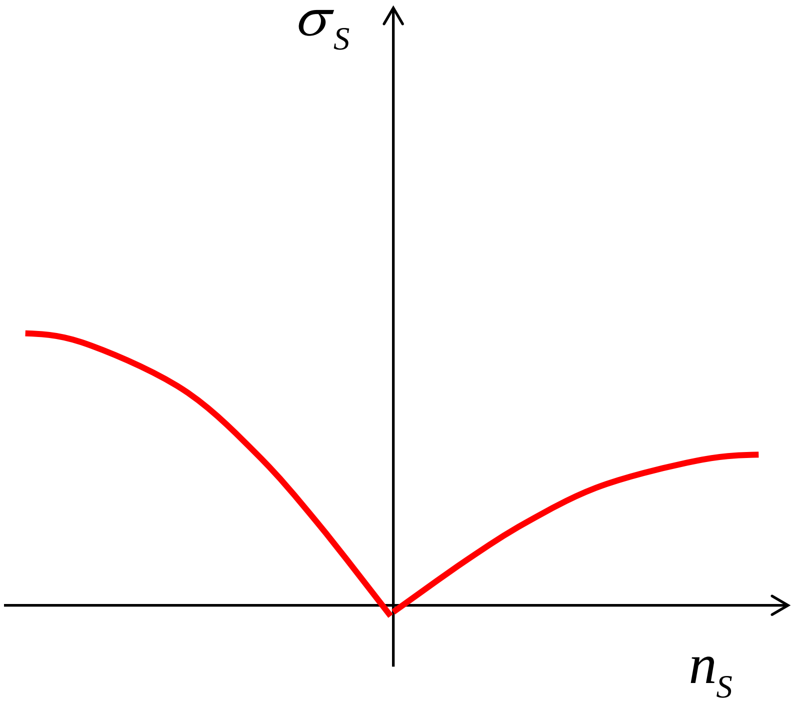
Charged-impurity (long-range) scattering.

Constant mobility.

Result is a combination of charged impurity and phonon scattering.

what about the contacts?





The contact resistance is voltage dependent. Contact can distort the characteristic and produce asymmetries between n- and p-type conduction.

Use 4-probe measurements!

outline

10.1 Graphene
10.2 Density of states and carrier density
10.3 Number of modes and conductance
10.4 Scattering
10.5 Conductance vs. carrier density
10.6 Discussion
10.7 Summary

mobility and effective mass

$$\sigma_s = \frac{2q^2}{h}\int \lambda(E)\frac{M(E)}{W}\left(-\frac{\partial f_0}{\partial E}\right)dE \approx \frac{2q^2}{h}\lambda(E_F)\frac{M(E_F)}{W} = n_S\, q\, \mu_n$$

$$\left.\begin{aligned}
&\frac{M(E_F)}{W} = \frac{2E_F}{\pi\hbar\upsilon_F} \\
&\lambda(E_F) = \frac{\pi}{2}\upsilon_F\tau_m(E_F) \\
&n_S = \frac{E_F^2}{\pi\hbar^2\upsilon_F^2}
\end{aligned}\right\} \quad \mu_n = \frac{q\tau_m(E_F)}{\left(E_F/\upsilon_F^2\right)}$$

$$\mu_n = \frac{q\tau_m(E_F)}{m^*}$$

$$m^* = \frac{E_F}{\upsilon_F^2}$$

$$m^* \equiv \frac{p}{\upsilon}$$

$$E(k) = \hbar k \upsilon_F$$

(Datta, *Lessons from Nanoscience*)

questions

1) Work out the Hall effect for graphene and show that it is the same as for parabolic bands, but with a different effective mass.

2) Graphene is said to have high thermal conductivity. Use the concepts from Lecture 9 to explain why.

(Datta, *Lessons from Nanoscience*)

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summary

1) The linear dispersion of graphene gives rise to several interesting features.

2) Near-equilibrium transport in this novel material is readily understood with the concepts developed in these lectures.

3) Several interesting apllications for graphene are currently being explored (e.g. transparent, flexible conductors, novel transistors, thermal management, supercapacitor electrodes, etc.

for more information

“Colloquium on Graphene Physics and Devices”
2009 NCN Summer School
http://nanohub.org/resources/7180

Dionisis Berdebes, Tony Low, and Mark Lundstrom. “Lecture Notes on Low Bias Transport in Graphene: An Introduction”

http://nanohub.org/resources/7436/download/Notes_on_low_field_transport_in_graphene.pdf

questions

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