PROBLEM SET #6
"Graphene"
due on 5/26/2023

Physics–172 / Applied Physics–272
Introduction to Solid State Physics
Spring quarter, 2023

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Problem 6.1 (Universal optical conductivity of graphene — **12 points**)**.** Electrons in graphene are described by effective Hamiltonian

$$\hat{H}_0 = v(\hat{\sigma}_x \hat{p}_x + \hat{\sigma}_y \hat{p}_y) = v \begin{pmatrix} 0 & \hat{p}_x - i\hat{p}_y \\ \hat{p}_x + i\hat{p}_y & 0 \end{pmatrix}$$

Here $v \sim 10^6$ m/s is Fermi velocity, Pauli matrices $\hat{\sigma}_i$ represent sub–lattice degree of freedom, and $\hat{\mathbf{p}}$ is momentum operator.

1. (**8 points**) Calculate conductivity of graphene $\sigma(\omega)$ at optical frequencies, assuming charge neutrality, $T = 0$ and no scattering $\tau \to \infty$.

   (a) (**1 point**) Find energies $\varepsilon_{s,\mathbf{p}}$ and eigenfunctions $|s, \mathbf{p}\rangle$ of Hamiltonian H_0. They are labeled by two quantum numbers: (quasi)momentum $\mathbf{p}$ and band index $s = \pm$. How should you normalize eigenfunctions $\langle s', \mathbf{p}' | s, \mathbf{p}\rangle =$?

   (b) (**2 points**) Compute velocity operator $\hat{\mathbf{v}} = \partial \hat{H}_0 / \partial \hat{\mathbf{p}}$.
   Hint. You should get 2×2 matrix in s–space.

   (c) (**5 points**) Using time–dependent perturbation theory compute linear response to applied electric field $\mathbf{E} \cos \omega t$, which you can treat as perturbation

   $$\hat{H} = \hat{H}_0 + \hat{V}, \quad \hat{V} = |e|(\mathbf{E} \cdot \mathbf{r})\theta(t) \cos \omega t.$$

   Hint. The most straight–forward way to tackle this calculation is with Kubo formula

   $$\mathbf{j}^{(1)}(t) = \frac{ie}{\hbar} \sum_s \int \frac{d\mathbf{p}}{(2\pi\hbar)^2} f(\varepsilon_{s,\mathbf{p}}) \left\langle s, \mathbf{p} \left| \int_0^t [\hat{V}_I(\tau), \hat{\mathbf{v}}_I(t)] d\tau \right| s, \mathbf{p} \right\rangle$$

   here operators $\hat{V}$ and $\hat{\mathbf{v}}$ are in interaction representation. Alternatively, you could approach this calculation old–fashioned way, and derive analog of [1, (13.37)]. It may be helpful to compare your calculation with what you can find in the literature [2].

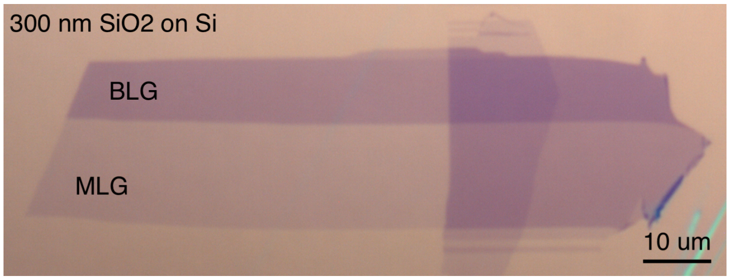
   You should obtain a beautiful result known as *universal optical conductivity* (remember to include spin and valley doubling in your calculation).

   $$\sigma(\omega) = \frac{e^2}{4\hbar}. \tag{6.1.1}$$

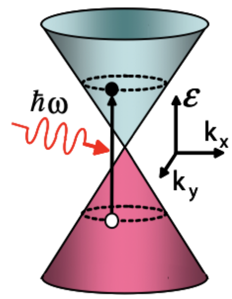
   Remarkably, this result holds true for real graphene as long as $\omega \gg \tau^{-1}$, T [3].

2. (**4 points**) Using result (6.1.1) calculate transmittance T for normal incidence on a single sheet of graphene in vacuum. What value do you expect for T? Take a look at the photo of graphene Fig 1a and check your intuition.

   Hint. Problem is fully described by Maxwell's equations, boundary conditions, continuity equation and Ohm's law $\mathbf{j} = \sigma_0 \delta(z) \mathbf{E}$.



(a) Optical photo of monolayer graphene (MLG) and bilayer graphene (BLG) on silicone substrate.



(b) Interaction of light with electrons in graphene (schematically) [3]

Figure 1: Illustrations for optical conductivity of graphene.

Problem 6.2 (Graphene conductivity — **10 points**). In this problem we will describe electron transport in graphene using relaxation time approximation [1, (13.22)]

$$e\mathbf{E} \cdot \frac{\partial f_{\mathbf{p}}}{\partial \mathbf{p}} = -\frac{f_{\mathbf{p}} - f_{\mathbf{p}}^{(0)}}{\tau}, \qquad \mathbf{j} = e \int_{\mathbf{p}} \mathbf{v}_{\mathbf{p}} f_{\mathbf{p}}, \qquad \mathbf{v}_{\mathbf{p}} = \frac{\partial \varepsilon_{\mathbf{p}}}{\partial \mathbf{p}}.$$

1. (**3 points**) Derive an expression for conductivity $\sigma = \sigma(\mu, T)$ within τ–approximation.
2. (**3 points**) Derive a relation between carrier density n and chemical potential μ.
3. (**4 points**) Compare your formula to experimental data presented on Fig. 2. How well this oversimplified model explains the data? Extract value of $\tau_{300\text{K}}$, would you say it's a short or a long relaxation time? Data is available online.

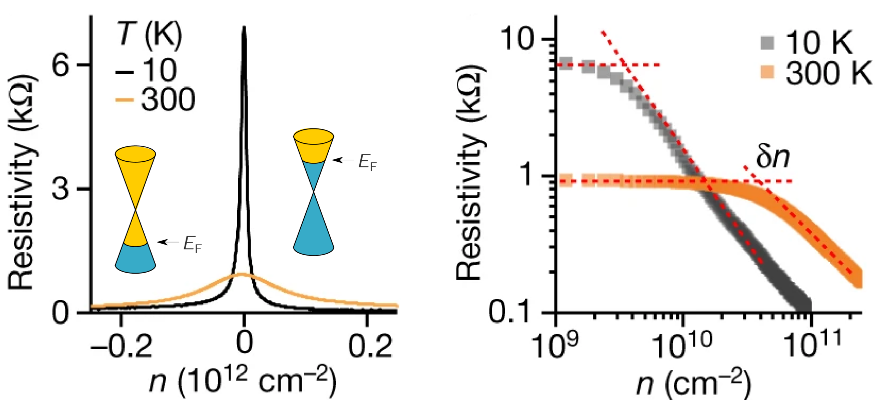


Figure 2: Resistivity of graphene vs carrier density [4].

Problem 6.3 (Landau levels in graphene — **10 points**)**.** Just like free electrons, quasielectrons in crystal experience Lorentz force in the presence of magnetic field, however, having non–free–electron–like dispersion introduces some differences. As you remember from classical mechanics, in the presence of magnetic field, we differentiate between canonical (generalized) momentum $\mathbf{p}$ and kinetic (covariant) momentum $\boldsymbol{\pi} = \mathbf{p} - \frac{e}{c}\mathbf{A}$, where electron charge $e = -|e|$ is negative. Similar to free–electron case, effective quantum Hamiltonian for quasielectrons in field, is achieved through canonical quantization of $\mathbf{p} = -i\hbar\nabla$, which is justified by Peierls substitution.

$$\hat{H} = v\left(\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{\pi}}\right) = v\left(\hat{\boldsymbol{\sigma}}, \hat{\mathbf{p}} + \frac{|e|}{c}\mathbf{A}\right), \qquad \mathbf{A} = (-By, 0, 0). \tag{6.3.1}$$

1. (**4 points**) Solve semi-classical equations[1] of motion for electrons in magnetic field directed perpendicular to graphene plane $\mathbf{B} = B\mathbf{e}_z$. Use Landau gauge.

$$\dot{\mathbf{r}} = \nabla_{\boldsymbol{\pi}}\varepsilon_{s,\boldsymbol{\pi}},$$
$$\dot{\boldsymbol{\pi}} = \frac{e}{c}[\dot{\mathbf{r}} \times \mathbf{B}].$$

   What is the expression for cyclotron frequency ω_c? Find Landau levels ε_n for electrons *and* holes using semiclassical quantization condition

$$\oint_{\varepsilon(\mathbf{p},\mathbf{r})=\varepsilon_n} \mathbf{p} \cdot d\mathbf{r} = 2\pi\hbar n.$$

2. (**6 points**) Solve stationary Schrödinger problem for Hamiltonian (6.3.1).

   (a) (**3 points**) Find energies ε_n and eigenvectors $\psi_{n,k}$. You can use harmonic oscillator functions (a.k.a normalized Hermite functions) $\psi_n^{\text{osc}}(x)$ in your answer.

$$\psi_n^{\text{osc}}(x) = \frac{e^{-x^2/2}H_n(x)}{\sqrt{2^n n!\sqrt{\pi}}}.$$

   Pay attention to zeroth Landau level. Which eigenvector does it correspond to?

   (b) (**2 points**) Compute energy difference between zeroth and first Landau level at $B = 1$ T. Express your answer in Kelvins.

   (c) (**1 point**) What is the degeneracy g_n of n–th Landau level?

3. (**0 points**) Find several low ($|n| < 10$) Landau levels numerically using method described in [6]. You once again have problems with the lowest Landau level, what is the reason for it this time?

Problem 6.4 (Graphene diode — **11 points**)**.** Consider n–p junction along x direction in graphene with symmetric electron and hole densities (see Fig.3) at absolute zero $T = 0$.

$$\hat{H}\psi = 0, \qquad \hat{H} = v\left(\hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{p}}\right) + e\varphi(x), \quad e < 0.$$

Junction potential $V(x)$ could be induced either through chemical doping or through electrostatic gating. In this problem we will consider two models for $V(x)$.

(a) Step–function $\varphi(x) = -V_0\,\text{sgn}(x)$, $V_0 > 0$.

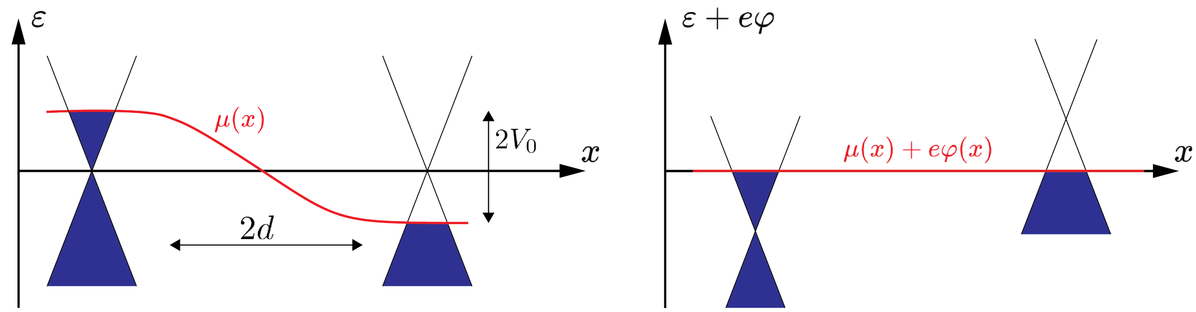


Figure 3: Energy profile in graphene n–p junction.

(b) Linear function $\varphi(|x| < d) = -V_0 x/d$ and $\varphi(|x| > d) = -V_0 \,\mathrm{sgn}(x)$, $k_F d \gg 1$.

For each of the two types of potential do the following:

1. (**6 points**) Find transmission coefficient for different incident angles $T(V_0, k_y)$ by solving standard scattering problem

$$\psi(x \to -\infty) = \psi_{\to}(x) + r \cdot \psi_{\leftarrow}(x), \qquad \psi(x \to +\infty) = t \cdot \psi_{\to}(x).$$

   Hint. For the case of linear potential (b) instead of solving the problem exactly, calculate transmission amplitude in WKB approximation.

$$t = e^{-S_T/\hbar}, \qquad S_T = \int_{-x_0}^{x_0} |q_\pm(x)| dx, \qquad q_\pm(x) = \pm\sqrt{\frac{e^2}{v^2}\varphi^2(x) - p_y^2},$$

   where $q(x)$ is semiclassical momentum, and integral for tunneling action is computed between classical turning points determined from $q(\pm x_0) = 0$.

2. (**5 points**) Calculate ballistic conductance of the diode using Landauer formula

$$G(V_0) = \frac{e^2}{2\pi\hbar} \sum_{k_y} T(V_0, k_y),$$

   and find IV characteristic of graphene diode $I = G(V_0 + V)V$, does it look as you expected? Plot current versus voltages in range -0.1 V to $+0.1$ V, assuming sample width $W = 10$ μm, symmetric concentration of carriers $n = p = 7.5 \cdot 10^{11}$ cm^{-2}, velocity $v = 10^6$ m/s and junction half–length $d = 50$ nm.

3. (**0 points**) Imagine an opening of a huge gap $\hat{H}_{\text{gapped}} = \hat{H} + \Delta\sigma_z$ with $\Delta = 72$ meV and the same carrier density. How does it change your answers?

References

[1] Neil Ashcroft and David Mermin. *Solid state physics.* Harcourt College Publishers, 1976.

[2] L. A. Falkovsky and A. A. Varlamov. Space-time dispersion of graphene conductivity. *The European Physical Journal B*, 56:281–284, 2007.

[1] We ignore contribution from the Berry's curvature[5] for simplicity.

[3] A. B. Kuzmenko, E. van Heumen, F. Carbone, and D. van der Marel. Universal optical conductance of graphite. *Phys. Rev. Lett.*, 100:117401, Mar 2008.

[4] Na Xin, James Lourembam, Piranavan Kumaravadivel, A. E. Kazantsev, Zefei Wu, Ciaran Mullan, Julien Barrier, Alexandra A. Geim, I. V. Grigorieva, Artem Mishchenko, et al. Giant magnetoresistance of dirac plasma in high-mobility graphene. *Nature*, 616(7956):270–274, 2023.

[5] P. Gosselin, H. Boumrar, and H. Mohrbach. Semiclassical quantization of electrons in magnetic fields: The generalized peierls substitution. *Europhysics Letters*, 84(5):50002, nov 2008.

[6] H. J. Korsch and M. Glück. Computing quantum eigenvalues made easy. *European Journal of Physics*, 23(4):413, jun 2002.