ECE 65600 (Electron Transport in Semiconductors) HW #6

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1) What are the special properties of a contact in the Landauer model?

a) Strong inelastic scattering keeps them near equilibrium.
b) Any electron incident upon the contact is completely absorbed (no reflections).
c) Each contact is described by its own Fermi level.
d) Contacts have a very large number of channels (modes) compared to the device.
e) All of the above.

The assumptions (a - d) describe the fundamental conditions for an ideal Landauer contact, as shown in Figure 1. These conditions ensure that the left and right contacts function as ideal reservoirs for electron transport in the channel. Therefore, **the correct answer is (e)**.

2) Which of the follow is true about the Landauer expression for current: $I=(2q/h)\int T(E)M(E)(f_1-f_2)dE$?

a) It applies to electrons in the conduction band.
b) It applies to electrons in the valence band.
c) It applies to holes in the valence band.
d) It applies to **both** electrons in the conduction band and holes in the valence band.
e) It applies to both electrons in the conduction band and electrons in the valence band.

The Landauer model describes n-type current flow as electron transport in the conduction band, and p-type current flow as electron transport in the valence band. The expressions are identical, differing only in the integration range. Please refer Figure 2 for details. In summary, **the correct answer is (e).**

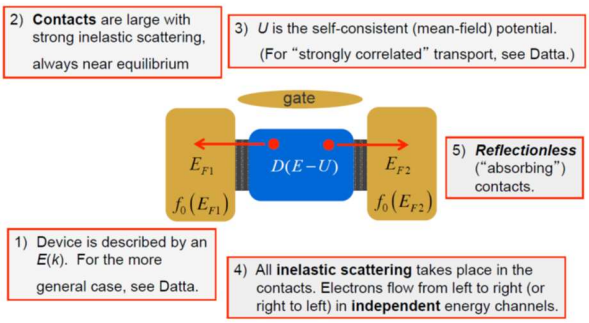

Figure 1. Conditions for the ideal Landauer contacts.

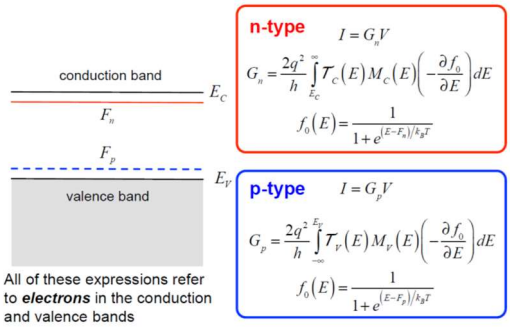

Figure 2. N-type and p-type Landauer transport.

3) What are the units of the quantity, $h\langle v_x^+(E)\rangle D(E)/4$? The units of $D(E)$ are J^{-1}.

a) Energy
b) One over energy
c) Ohms
d) One over Ohms or Siemens.
e) The quantity is unitless.

I believe that $D(E)$ denotes the 1D DOS, which has units of $[J^{-1}\cdot m^{-1}]$; since it is the *density* of states in *energy* space, its units should be normalized by the energy and hyper-volume (in this case, length). Then, the Planck constant, velocity, and 1D DOS has units of $[J\cdot s]$, $[m\cdot s^{-1}]$, and $[J^{-1}\cdot m^{-1}]$, respectively. By using them, one

can compute the units of $M(E)$ as follows:

$$[M] = [\mathrm{J}\cdot\mathrm{s}]\left[\frac{\mathrm{m}}{\mathrm{s}}\right]\left[\frac{1}{J\cdot\mathrm{m}}\right] \Longrightarrow \text{unitless} \tag{1}$$

Therefore, $M(E)$ is a dimension-less quantity, thus **the correct answer is (e).**

4) What is meant by the term "near-equilibrium" transport?

a) The contacts stay very close to equilibrium.
b) The Fermi level in the contact is close to its equilibrium value.
c) The Fermi levels of the two contacts, f_1 and f_2, can be replaced by the equilibrium Fermi level.
d) The difference in Fermi levels between the two contacts can be replaced by a first order Taylor series expansion of $f_1 - f_2$.
e) The temperature of the two contacts is the same.

"Near-equilibrium transport" refers to a condition where current flows due to a slight difference in the Fermi levels between the right and left contacts. Mathematically, it means that the difference in Fermi Dirac distributions in these contacts, i.e., the Fermi window $f_1 - f_2$, can be approximated by using the first order Taylor expansion, i.e., $f_2 \approx f_1 + (\partial f_1/\partial E)(qV) \Longrightarrow f_1 - f_2 \approx (-\partial f_1/\partial E)(qV)$. **Thus, the correct answer is (d).**

5) Consider a small nano-device under bias with a steady-state current flowing. Which of the following is true?

a) One contact tries to fill states in the device and the other one tries to empty them.
b) Both contacts try to fill states in the device.
c) Both contacts try to empty states in the device.
d) All of the above.
e) None of the above.

The device is biased thus current flows. The electron that exits from one contact (the left or "source" contact) must travel the channel and enter the other contact (the right or "drain" contact). **Thus, the correct answer is (a);** the source contact tries to fill states in the device, and the other one tries to empty them. Please refer Figure 3 for details.

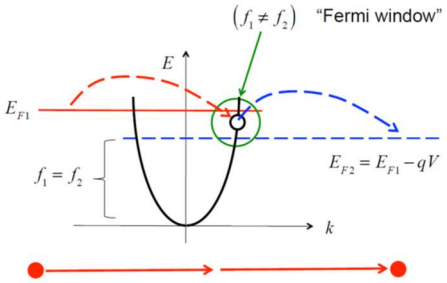

Figure 3. Visualization of electron transport.

6) Mathematically, the number of modes (channels) at energy, E, is proportional to what?

a) The density of states.
b) The velocity.
c) The density of states times velocity.
d) The density of states divided by velocity.
e) The deBroglie wavelength.

The number of modes is given by $h\langle v_x^+(E)\rangle D(E)/4$, i.e., the density of states times velocity, **thus the correct answer is (c).**

7) How is the transmission, $\mathcal{T}$, related to the mean-free-path for backscattering, λ, and the length of the resistor, L?

a) $\mathcal{T} = e^{-L/\lambda}$.
b) $\mathcal{T} = e^{+L/\lambda}$.
c) $\mathcal{T} = \lambda/L$.
d) $\mathcal{T} = L/\lambda$.
e) $\mathcal{T} = \lambda/(\lambda + L)$.

The transmission $T = \lambda/(\lambda + L)$ is a unified expression that can describe diffusive, ballistic, and quasi ballistic transports as shown in Figure 4. **Thus, the correct answer is (e).**

8) For parabolic band semiconductors, $M(E)$ is independent of energy (above the bottom of the conduction band) for which of the following cases?

a) 1D
b) 2D
c) 3D
d) 1D and 2D
e) 2D and 3D

Figure 5 shows the computed $M(E)$ profiles for 1D, 2D, and 3D cases. The 1D case is a unit function in the energy space, meaning the 1D $M(E)$ is independent of energy. **Thus, the correct answer is (a).**

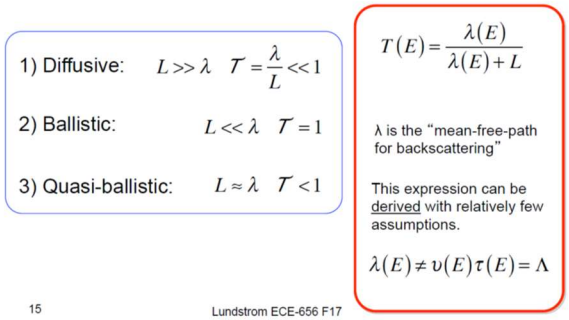

Figure 4. Transmission model based on the mean free path λ and device length L.

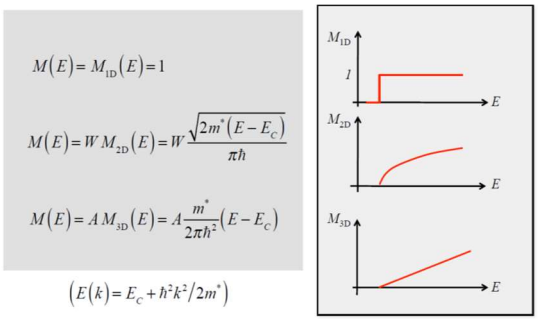

Figure 5. Comparison of $M(E)$ for 1D, 2D, and 3D cases, with parabolic energy bands.

3) Determine the limits of integration, E_1 and E_2, for the integral in the Landauer expression:

$$I = (2q/h)\int_{E_1}^{E_2} \mathcal{T}(E) M(E)(f_1 - f_2)\,dE$$

for the case of $T = 0$ K. Assume that contact one is grounded and that a positive voltage (not necessarily small) has been applied to contact 2.

For $T = 0K$, the Fermi window $f_1 - f_2$ is simply given by a rectangular filter, as shown in Figure 6. It equals 1 if E lies within the difference between the two contact Fermi levels, and 0 otherwise, thus the integration range is also determined based on the Fermi levels. Let the Fermi level of the contact 1 be 0; then the Fermi level of the contact 2 is simply given by qV. **Therefore, the integration range extends from $E_1 = qV$ to $E_2 = 0$** (because a positive bias is applied, qV is negative and smaller than 0).

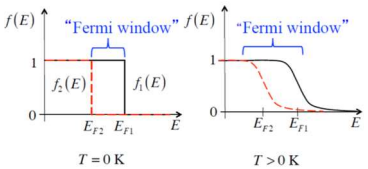

Figure 6. Fermi window at $T = 0K$ and $T > 0K$.

4) The ballistic conductance is often derived from a k-space treatment, which writes the current from left to right as

$$I^{+} = \frac{1}{L}\sum_{k>0} q v_x f_0(E_{F1})$$

and the current from right to left as

$$I^{-} = \frac{1}{L}\sum_{k<0} q v_x f_0(E_{F2})$$

The net current is the difference between the two. In the ballistic limit, the Landauer expression for the current is

$$I = (2q/h)\int_{E_1}^{E_2} M(E)(f_1 - f_2)dE$$

4a) Assume parabolic energy bands, evaluate the net current from the k-space approach, and show that it is the same as the Landauer expression.

4b) Assume parabolic energy bands, but now assume **2D electrons**. Evaluate the net current from the k-space approach, and show that it is the same as the Landauer expression.

4c) Assume parabolic energy bands, but now assume 3D electrons. Evaluate the net current from the k-space approach, and show that it is the same as the Landauer expression.

Without loss of generality, $E_C = 0$, $g_s = 2$, and $g_v = 1$ are assumed for sake of simplicity.

(4a) The 1D Landauer equation is given by

$$I_{L,1\mathrm{D}} = \frac{2q}{h}\int dE M(E)(f_1 - f_2) = \frac{2q}{h}\int dE(f_1 - f_2), \tag{2}$$

because the number of modes $M(E)$ for 1D is equal to 1, as shown in Figure 5. Next, let me derive the ballistic current from the k-space approach. For 1D electrons, $\sum_k \Longrightarrow 2\frac{L}{2\pi}\int 2dk$ and $v_x = \frac{1}{\hbar}\frac{\partial E}{\partial k}$. From this, I_+ is expressed as

$$I_{+,1\mathrm{D}} = \frac{1}{L}\sum_{k>0} q v_x f_1 = \frac{1}{L}\frac{L}{\pi}\int \left(2dk \cdot \frac{1}{2}\right) q \frac{1}{\hbar}\frac{\partial E}{\partial k} f_1 = \frac{q}{\pi\hbar}\int dE f_1 = \frac{2q}{h}\int dE f_1, \tag{3}$$

where $1/2$ is multiplied to $2dk$ to consider $k > 0$ only. Similarly, I_- is expressed as

$$I_{-,1\mathrm{D}} = \frac{2q}{h}\int dE f_2. \tag{4}$$

Therefore, the net current derived from the k-space approach is given by

$$I_{k,1\mathrm{D}} = I_{+,1\mathrm{D}} - I_{-,1\mathrm{D}} = \frac{2q}{h}\int dE(f_1 - f_2). \tag{5}$$

Thus, one can conclude

$$\boxed{I_{k,1\mathrm{D}} = \frac{2q}{h}\int dE(f_1 - f_2) = I_{L,1\mathrm{D}}}. \tag{6}$$

(4b) The 2D Landauer equation is given by

$$I_{L,2\mathrm{D}} = \frac{2q}{h}\int dE M(E)(f_1 - f_2) = \frac{2q}{2\pi\hbar}\int dE\left(W\frac{\sqrt{2m^*E}}{\pi\hbar}\right)(f_1 - f_2) = \frac{q\sqrt{2m^*}}{\pi^2\hbar^2}W\int dE\sqrt{E}(f_1 - f_2), \tag{7}$$

by using the $M(E)$ for 2D shown in Figure 5. Next, to derive the ballistic current from the k-space approach, let me consider $\sum_k \Longrightarrow 2\frac{L}{2\pi}\frac{W}{2\pi}\int\int kdk\,d\theta$ and $v_x = \frac{1}{\hbar}\frac{\partial E}{\partial k_x} = \frac{1}{\hbar}\frac{\partial}{\partial k_x}\left(\frac{\hbar^2}{2m^*}\left(k_x^2+k_y^2\right)\right) = \frac{\hbar}{m^*}k_x = \frac{\hbar}{m^*}k\cos\theta$. Then,

$$\begin{aligned} I_{+,2\mathrm{D}} &= \frac{1}{L}\sum_{k_x>0,k_y} qv_x f_1 = \frac{W}{2\pi^2}\int\int f_1\frac{\hbar}{m^*}q(k\cos\theta)kdkd\theta = \frac{qW}{2\pi^2}\frac{\hbar}{m^*}\int k^2dkf_1\int_{-\pi/2}^{\pi/2}\cos\theta d\theta \\ &= \frac{qW}{\pi^2}\frac{\hbar}{m^*}\int k^2dkf_1, \end{aligned} \tag{8}$$

where the integration range in θ space is limited to $[-\pi/2,\pi/2]$ in order to consider only $k_x>0$. Now, using $E=\frac{\hbar^2k^2}{2m^*}\Longrightarrow k^2=\frac{2m^*}{\hbar^2}E, k=\frac{\sqrt{2m^*}}{\hbar}\sqrt{E}$ and $kdk=\frac{m^*}{\hbar^2}dE$, one can simplify (8) as follows:

$$I_{+,2D} = \frac{qW}{\pi^2}\frac{\cancel{\hbar}}{\cancel{m^*}}\int\frac{\sqrt{2m^*}}{\cancel{\hbar}}\sqrt{E}\,\frac{\cancel{m^*}}{\hbar^2}dEf_1 = \frac{qW}{\pi^2}\frac{\sqrt{2m^*}}{\hbar^2}\int\sqrt{E}\,dEf_1. \tag{9}$$

Similarly, I_{-} is expressed as

$$I_{-,2D} = \frac{qW}{\pi^2}\frac{\sqrt{2m^*}}{\hbar^2}\int\sqrt{E}\,dEf_2. \tag{10}$$

Therefore, the net current derived from the *k*-space approach is given by

$$I_{k,2\mathrm{D}} = I_+ - I_- = \frac{q\sqrt{2m^*}}{\pi^2\hbar^2}W\int\sqrt{E}\,dE(f_1-f_2). \tag{11}$$

Thus, one can conclude

$$\boxed{I_{k,2\mathrm{D}} = \frac{q\sqrt{2m^*}}{\pi^2\hbar^2}W\int\sqrt{E}\,dE(f_1-f_2) = I_{L,2\mathrm{D}}}. \tag{12}$$

(4c) The 3D Landauer equation is given by

$$I_{L,3\mathrm{D}} = \frac{2q}{h}\int dEM(E)(f_1-f_2) = \frac{2q}{2\pi\hbar}\int dE\left(A\frac{m^*}{2\pi\hbar^2}E\right)(f_1-f_2) = \frac{qm^*}{2\pi^2\hbar^3}A\int EdE(f_1-f_2), \tag{13}$$

by using the $M(E)$ for 2D shown in Figure 5. Next, to derive the ballistic current from the k-space approach, let me consider $\sum_k \Longrightarrow 2\frac{L}{2\pi}\frac{W}{2\pi}\frac{H}{2\pi}\int\int\int k^2\sin\theta dkd\theta d\varphi$ and $v_x = \frac{1}{\hbar}\frac{\partial E}{\partial k_x} = \frac{1}{\hbar}\frac{\partial}{\partial k_x}\left(\frac{\hbar^2}{2m^*}\left(k_x^2+k_y^2+k_z^2\right)\right) = \frac{\hbar}{m^*}k_x = \frac{\hbar}{m^*}k\sin\theta\cos\varphi$. Then,

$$\begin{aligned} I_{+,3\mathrm{D}} &= \frac{1}{L}\sum_{k_x>0,k_y,k_z} qv_x f_1 = \frac{(WH)}{4\pi^3}\int\int\int f_1 q\left(\frac{\hbar}{m^*}k\sin\theta\cos\varphi\right)k^2\sin\theta dkd\theta d\varphi \\ &= \frac{A}{4\pi^3}\frac{q\hbar}{m^*}\int\int\int f_1k^3\sin^2\theta\cos\varphi dkd\theta d\varphi \\ &= \frac{A}{4\pi^3}\frac{q\hbar}{m^*}\underbrace{\int_{-\pi/2}^{\pi/2}d\varphi\cos\varphi}_{=2}\underbrace{\int_0^{\pi}d\theta\sin^2\theta}_{=\pi/2}\int f_1k^3dk = \frac{A}{4\pi^2}\frac{q\hbar}{m^*}\int f_1k^3dk, \end{aligned} \tag{14}$$

where the integration range in φ space is limited to $[-\pi/2,\pi/2]$ in order to consider only $k_x>0$. Now, using $E=\frac{\hbar^2k^2}{2m^*}\Longrightarrow k^2=\frac{2m^*}{\hbar^2}E$ and $kdk=\frac{m^*}{\hbar^2}dE$, one can simplify (14) as follows:

$$I_{+,3\mathrm{D}} = \frac{A}{4\pi^2}\frac{q\cancel{\hbar}}{\cancel{m^*}}\int f_1\frac{2\cancel{m^*}}{\cancel{\hbar^2}}E\frac{m^*}{\hbar^2}dE = \frac{A}{2\pi^2}\frac{qm^*}{\hbar^3}\int f_1EdE. \tag{15}$$

Similarly, I_{-} is expressed as

$$I_{-,3\mathrm{D}} = \frac{A}{2\pi^2}\frac{qm^*}{\hbar^3}\int f_2 E dE. \tag{16}$$

Therefore, the net current derived from the *k*-space approach is given by

$$I_{k,3\mathrm{D}} = I_{+} - I_{-} = \frac{qm^*}{2\pi^2\hbar^3} A \int E dE (f_1 - f_2). \tag{17}$$

Thus, one can conclude

$$\boxed{I_{k,3\mathrm{D}} = \frac{qm^*}{2\pi^2\hbar^3} A \int E dE (f_1 - f_2) = I_{L,3\mathrm{D}}}. \tag{18}$$

5) **The quantity,**

$$\langle M \rangle = \int_{E_C}^{\infty} M(E)\left(-\frac{\partial f_0}{\partial E}\right) dE$$

is the number of conduction band channels in the Fermi-Window. Answer the following questions.

5a) **Evaluate $\langle M \rangle$ for an arbitrary temperature and location of the Fermi level assuming a 2D semiconductor with parabolic energy bands.**

5b) **Evaluate $\langle M \rangle$ for an arbitrary temperature and location of the Fermi level above the Dirac point, E_D, assuming graphene.**

5c) **Assume that $E_F = E_C + 0.1\,\mathrm{eV} = E_D + 0.1\,\mathrm{eV}$. For 5a), assume Si with $m^* = 0.19 m_0$ and a valley degeneracy of 2. For 5b), assume graphene parameters, $\upsilon_F = 10^8$ cm/s and a valley degeneracy of 2. Compare the numerical values of $\langle M \rangle$ for these two cases assuming T = 300 K.**

(5a) By using the definition of $\langle M \rangle$ given in the problem and $M(E)$ for 2D semiconductors shown in Figure 5, the full expression of $\langle M \rangle$ is

$$\langle M \rangle = \int_{E_C}^{\infty} \left(W\frac{\sqrt{2m^*(E-E_C)}}{\pi\hbar}\right)\left(-\frac{\partial f_0}{\partial E}\right) dE = W\frac{\sqrt{2m^*}}{\pi\hbar}\int_{E_C}^{\infty} \sqrt{E-E_C}\left(-\frac{\partial f_0}{\partial E}\right) dE. \tag{19}$$

For the sake of simplicity, let $W\frac{\sqrt{2m^*}}{\pi\hbar} = C$. Note that for the Fermi-Dirac distribution, $-\partial f_0/\partial E = \partial f_0/\partial E_F$ holds. Using this identity, the above becomes

$$\langle M \rangle = C\int_{E_C}^{\infty} \left(\sqrt{E-E_C}\right)\left(\frac{\partial f_0}{\partial E_F}\right) dE = C\frac{\partial}{\partial E_F}\int_{E_C}^{\infty} \left(\sqrt{E-E_C}\right) f_0\, dE = C\frac{\partial}{\partial E_F}\int_{E_C}^{\infty} \frac{\sqrt{E-E_C}}{1+\exp((E-E_F)/k_BT)} dE. \tag{20}$$

To covert this equation as a usual Fermi-Dirac integral form, let $\eta = (E-E_C)/k_BT$ and $\eta_F = (E_F - E_C)/k_BT$. Then, (20) is equal to

$$\langle M \rangle = C\frac{\partial}{\partial E_F}\int_0^{\infty} \frac{\sqrt{k_BT\eta}}{1+\exp(\eta-\eta_F)} k_BT d\eta = C\sqrt{k_BT}\frac{\partial}{\partial \eta_F}\int_0^{\infty} \frac{\sqrt{\eta}}{1+\exp(\eta-\eta_F)} d\eta. \tag{21}$$

Note that for the Fermi-Dirac integral, $\int_0^\infty \frac{\eta^j}{1+\exp(\eta-\eta_F)}d\eta = \Gamma(j+1)\mathcal{F}_j$ and $\frac{\partial}{\partial\eta_F}\mathcal{F}_j = \mathcal{F}_{j-1}$. Thus (21) is a derivative of the Fermi-Dirac integral of order 1/2 and should be the Fermi-Dirac integral of order – 1/2. Because $\Gamma(1/2+1) = \frac{\sqrt{\pi}}{2}$, (21) is finally given by

$$\langle M\rangle = C\sqrt{k_BT}\frac{\partial}{\partial\eta_F}\left(\frac{\sqrt{\pi}}{2}\mathcal{F}_{1/2}\right) = W\frac{\sqrt{2m^*}}{\pi\hbar}\frac{\sqrt{\pi k_BT}}{2}\mathcal{F}_{-1/2} = W\frac{\sqrt{2\pi m^*k_BT}}{2\pi\hbar}\mathcal{F}_{-1/2} = \boxed{W\frac{\sqrt{2\pi m^*k_BT}}{h}\mathcal{F}_{-1/2}}. \quad (22)$$

(5b) From the lecture note, $M(E)$ for graphene is given by

$$M(E) = W\frac{2E}{\pi\hbar v_F}, \quad (23)$$

for the case where the Fermi level is above the Dirac point, i.e., $E > 0$. Then, similar to the previous case, the full expression of $\langle M\rangle$ is

$$\langle M\rangle = \int_0^\infty \left(W\frac{2E}{\pi\hbar v_F}\right)\left(-\frac{\partial f_0}{\partial E}\right)dE = W\frac{2}{\pi\hbar v_F}\int_0^\infty E\left(-\frac{\partial f_0}{\partial E}\right)dE. \quad (24)$$

Again, let $W\frac{2}{\pi\hbar v_F} = C$ for simplicity. Using the technique $-\partial f_0/\partial E = \partial f_0/\partial E_F$ gives

$$\langle M\rangle = C\int_0^\infty E\frac{\partial f_0}{\partial E_F}dE = C\frac{\partial}{\partial E_F}\int_0^\infty Ef_0\,dE = C\frac{\partial}{\partial E_F}\int_0^\infty \frac{E}{1+\exp((E-E_F)/k_BT)}dE. \quad (25)$$

To covert this equation as a usual Fermi-Dirac integral form, let $\eta = E/k_BT$ and $\eta_F = E_F/k_BT$, then (25) is equal to

$$\langle M\rangle = C\frac{\partial}{\partial E_F}\int_0^\infty \frac{k_BT\eta}{1+\exp(\eta-\eta_F)}k_BTd\eta = Ck_BT\frac{\partial}{\partial\eta_F}\int_0^\infty \frac{\eta}{1+\exp(\eta-\eta_F)}d\eta. \quad (26)$$

Again, this equation can be considered as the derivative of the Fermi-Dirac integral of order 1, which results in the Fermi-Dirac integral of order 0, as follows:

$$\langle M\rangle = Ck_BT\frac{\partial}{\partial\eta_F}\mathcal{F}_1 = Ck_BT\mathcal{F}_0 = \boxed{W\frac{2k_BT}{\pi\hbar v_F}\mathcal{F}_0}. \quad (27)$$

Although (27) already provides a compact expression for $\langle M\rangle$ in graphene, further progress can be made since the Fermi-Dirac integral of order 0 is analytically solvable.

$$\langle M\rangle = W\frac{2k_BT}{\pi\hbar v_F}\mathcal{F}_0 = W\frac{2k_BT}{\pi\hbar v_F}\ln(1+\exp(\eta_F)) = \boxed{W\frac{2k_BT}{\pi\hbar v_F}\ln\left(1+\exp\left(\frac{E_F}{k_BT}\right)\right)}. \quad (28)$$

(5c) First, let me consider the normalized $\langle M\rangle$, thus neglecting the width W. Note that the expression (22) is derived with $g_v = 1$ while the expression (22) is derived with $g_v = 2$. So, to satisfy the statement of the problem, (22) should be multiplied by 2. Using these expressions and given constants, the numerical results are given by

$$\langle M\rangle_{\mathrm{Si}} = \left.\frac{2\sqrt{2\pi m^*k_BT}}{h}\right|_{m^*=0.19,T=300\mathrm{K}}\mathcal{F}_{-1/2}(\eta_F = 0.1/0.0259) = \boxed{4.35\times10^8[\mathrm{m}^{-1}]}, \quad (29)$$

where $\mathcal{F}_{-1/2}$ is computed by using [3], and

$$\langle M\rangle_{\mathrm{graphne}} = \left.\frac{2k_BT}{\pi\hbar v_F}\right|_{v_F=10^6\mathrm{m/s},T=300\mathrm{K}}\ln\left(1+\exp\left(\frac{0.1}{0.0259}\right)\right) = \boxed{9.7\times10^7[\mathrm{m}^{-1}]}. \quad (30)$$

Therefore, the number of modes of Si is approximately four times larger than that of graphene.

References (other than the course material)

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