

Appendix

A Density of State

A central property of electronic materials is the Density of States (DOS) $N(E)$, which informs us of the density of mobile electrons or holes present in the solid at a given temperature. Formally, in two dimensions, the total number of states available between energy E and an interval dE is given by the differential area in k -space dA divided by the area of one k -state. Mathematically, this is equivalent to

$$N(E) = g_S g_V \frac{dA}{(2\pi)^2/\Omega}, \quad (\text{A.1})$$

where $g_S = 2$ is the spin degeneracy, g_V is the zone degeneracy, and Ω is the area of the lattice. There are six equivalent K-points, and each K-point is shared by three hexagons; therefore, $g_V = 2$ for graphene. To determine dA , let us consider a circle of constant energy in k -space. The perimeter of the circle is $2\pi k$ and the differential area obtained by an incremental increase of the radius by dk is $2\pi k dk$. Therefore, the DOS, which is always a positive value or zero, is

$$N(E_k) = \frac{2}{\pi} \left| k \left(\frac{dE}{dk} \right)^{-1} \right|, \quad (\text{A.2})$$

where $N(E)$ has been normalized to the Ω . To obtain the DOS for Graphene Systems, we first use the energy dispersion relations calculated within the Dirac approximation in Eq. (A.2);

$$E_k^{\text{MLG}} = \gamma k \quad \Rightarrow \quad \frac{dE}{dk} = \gamma \quad \& \quad N^{\text{MLG}}(E_k) = \frac{2k}{\pi\gamma} \quad (\text{A.3})$$

$$E_k^{\text{BLG}} = \frac{\hbar^2 k^2}{2m} \quad \Rightarrow \quad \frac{dE}{dk} = \frac{\hbar^2 k}{m} \quad \& \quad N^{\text{BLG}}(E_k) = \frac{2m}{\pi\hbar^2} \quad (\text{A.4})$$

$$E_k^{\text{MLGG}} = \sqrt{(\gamma k)^2 + \Delta^2} \quad \Rightarrow \quad \frac{dE}{dk} = \frac{\gamma^2 k}{\sqrt{(\gamma k)^2 + \Delta^2}} \quad \& \quad N^{\text{MLGG}}(E_k) = \frac{\sqrt{(\gamma k)^2 + \Delta^2}}{\pi\gamma^2} \quad (\text{A.5})$$

B Carrier Density

The electron carrier density is simply the number of states that are occupied per unit area at a given temperature. The occupation probability for electrons at finite temperatures is given by the Fermi–Dirac distribution, $f(E) = (1 + e^{(E-\mu_c)/k_B T})^{-1}$. The net carrier density $|n_e - n_p| = n_c$, where n_e stands for the filled states for $E > 0$, and n_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:

$$|n_e - n_p| = n_c = \int_0^\infty dE N(E) f(E) - \int_{-\infty}^0 dE N(E) (1 - f(E)), \quad (\text{B.1})$$

where $N(E)$ is the density of state for Graphene Systems.

[I] Monolayer Graphene (MLG)

The net Carrier density for MLG can be evaluated from Eqs. (A.3) & (B.1);

$$n_c^{\text{MLG}} = \frac{2}{\pi \gamma^2} \left(\int_0^\infty dE \frac{E^{\text{MLG}}}{1 + e^{(E-\mu_c)/k_B T}} - \int_{-\infty}^0 dE \frac{E^{\text{MLG}} e^{(E^{\text{MLG}} - \mu_c)/k_B T}}{1 + e^{(E-\mu_c)/k_B T}} \right) \quad (\text{B.2})$$

$$n_c^{\text{MLG}} = \frac{2}{\pi \gamma^2} \left(\int_0^\infty dE \frac{E^{\text{MLG}}}{1 + e^{(E-\mu_c)/k_B T}} - \int_0^\infty dE \frac{E^{\text{MLG}}}{1 + e^{(E+\mu_c)/k_B T}} \right) \quad (\text{B.3})$$

At zero temperature, chemical potential set to Fermi energy, i.e. $\mu_c = E_f^{\text{MLG}} = \gamma k_f$. Now we can easy to extract from relation (B.3) by making the following substitution,

$$\frac{1}{1 + e^{(E^{\text{MLG}} - E_f^{\text{MLG}})/k_B T}} \Big|_{T=0} = 1 - \text{step}(E^{\text{MLG}} - E_f^{\text{MLG}}), \quad (\text{B.4})$$

which will lead to the following

$$n_c^{\text{MLG}} = \frac{2}{\pi \gamma^2} \int_0^\infty dE^{\text{MLG}} E^{\text{MLG}} \left[\left(1 - \text{step}(E^{\text{MLG}} - E_f^{\text{MLG}}) \right) - \left(1 - \text{step}(E^{\text{MLG}} + E_f^{\text{MLG}}) \right) \right] \quad (\text{B.5})$$

Finally, the net carrier density in MLG is define as

$$n_c^{\text{MLG}} = \frac{(E_f^{\text{MLG}})^2}{\pi\gamma^2}. \quad (\text{B.6})$$

[II] Bilayer Graphene (BLG)

The net carrier density for BLG can be evaluated from Eqs. (A.4) & (B.1);

$$n_c^{\text{BLG}} = \int_0^\infty dE^{\text{BLG}} N^{\text{BLG}}(E)f(E) - \int_{-\infty}^0 dE^{\text{BLG}} N^{\text{BLG}}(E)(1 - f(E)) \quad (\text{B.7})$$

$$n_c^{\text{BLG}} = \frac{2m}{\pi\hbar^2} \left(\int_0^\infty dE^{\text{BLG}} \frac{1}{1+e^{(E^{\text{BLG}}-\mu_c)/k_B T}} - \int_{-\infty}^0 dE^{\text{BLG}} \frac{e^{(E^{\text{BLG}}-\mu_c)/k_B T}}{1+e^{(E^{\text{BLG}}-\mu_c)/k_B T}} \right) \quad (\text{B.8})$$

$$n_c^{\text{BLG}} = \frac{2m}{\pi\hbar^2} \left(\int_0^\infty dE^{\text{BLG}} \frac{1}{1+e^{(E^{\text{BLG}}-\mu_c)/k_B T}} - \int_0^\infty dE^{\text{BLG}} \frac{1}{1+e^{(E^{\text{BLG}}+\mu_c)/k_B T}} \right) \quad (\text{B.9})$$

At zero temperature, chemical potential set to Fermi energy, i.e. $\mu_c = E_f^{\text{BLG}} = \hbar^2 k_f^2 / 2m$. Now we can easy to extract from Eqs. (B.9) and (B.3) which will lead to the following

$$n_c^{\text{BLG}} = \frac{2m}{\pi\hbar^2} \int_0^\infty dE^{\text{BLG}} \left[\left(1 - \text{step}(E^{\text{BLG}} - E_f^{\text{BLG}}) \right) - \left(1 - \text{step}(E^{\text{BLG}} + E_f^{\text{BLG}}) \right) \right]. \quad (\text{B.10})$$

Finally, the net carrier density in BLG is define as

$$n_c^{\text{BLG}} = \frac{2mE_f^{\text{BLG}}}{\pi\hbar^2}. \quad (\text{B.11})$$

[III] Monolayer Gapped Graphene (MLGG)

The net carrier density for MLLG can be calculated similarly to that in MLG except the lower integration limit in Eq. (B.1) should be depend on Δ since the density of states is proportional to energy at $|E| > |\Delta|$ and is zero at $|E| < |\Delta|$. Now rewrite Eq. (B.1) with modification as

$$n_c^{\text{MLGG}} = \int_\Delta^\infty dE N^{\text{MLGG}}(E)f(E) - \int_{-\infty}^{-\Delta} dE N^{\text{MLGG}}(E)(1 - f(E)) \quad (\text{B.12})$$

$$n_c^{\text{MLGG}} = \frac{2}{\pi\gamma^2} \left(\int_\Delta^\infty dE \frac{\sqrt{E^2 + \Delta^2}}{1+e^{(E-\mu_c)/k_B T}} - \int_{-\infty}^{-\Delta} dE \frac{\sqrt{E^2 + \Delta^2} e^{(E-\mu_c)/k_B T}}{1+e^{(E-\mu_c)/k_B T}} \right) \quad (\text{B.13})$$

At zero temperature, chemical potential set to Fermi energy, i.e. $\mu_c = \mu_f = \sqrt{(\gamma k_f)^2 + \Delta^2}$.

The net carrier density in MLGG can be calculated similarly to the above and it is define as

$$n_c^{\text{MLGG}} = \frac{E_f^2}{\pi \gamma^2}. \quad (\text{B.14})$$

C Chemical Potential

The finite-temperature chemical potential μ_c is determined by the conservation of the total electron charge density as

$$n_c = \int_0^\infty dE \frac{N(E)}{1+e^{(E-\mu_c)/k_B T}} - \int_0^\infty dE \frac{N(E)}{1+e^{(E+\mu_c)/k_B T}}. \quad (\text{B.15})$$

[I] Monolayer Graphene (MLG)

Finite temperature chemical potential ($\mu_c^{\text{MLG}}(T)$) can be evaluated from Eqs. (B.6) & (B.15);

$$\frac{(E_f^{\text{MLG}})^2}{\pi \gamma^2} = \frac{2}{\pi \gamma^2} \left(\int_0^\infty dE^{\text{MLG}} \frac{E^{\text{MLG}}}{1+e^{(E^{\text{MLG}}-\mu_c^{\text{MLG}})/k_B T}} - \int_0^\infty dE^{\text{MLG}} \frac{E^{\text{MLG}}}{1+e^{(E^{\text{MLG}}+\mu_c^{\text{MLG}})/k_B T}} \right). \quad (\text{B.16})$$

Using the scaled parameter; $\frac{E^{\text{MLG}}}{E_f^{\text{MLG}}} = x$, $\frac{\mu_c}{E_f^{\text{MLG}}} = s$ and $\frac{T}{T_f} = y$, Eq.(B.16) can be written as

$$\frac{1}{2} \left(\frac{1}{y} \right)^2 = \int_0^\infty dx \frac{x}{1+e^{(x-s)/y}} - \int_0^\infty dx \frac{x}{1+e^{(x+s)/y}}. \quad (\text{B.17})$$

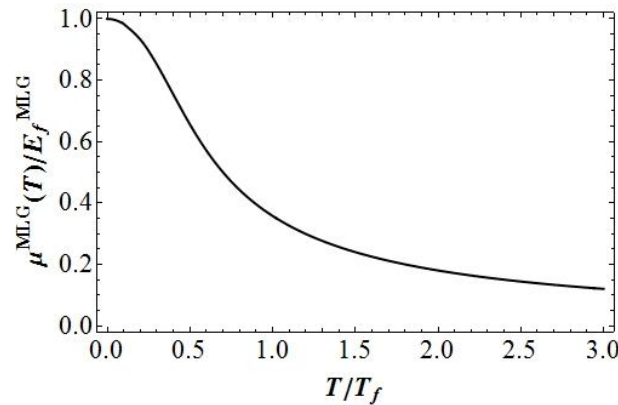


Figure A.1: The chemical potential of MLG as a function of temperature.

Equation (B.17) is plotted in Figure A.1 which shows that variation of $\mu_c^{\text{MLG}}(T)$ as a function of temperature.

[II] Bilayer Graphene (BLG)

Finite temperature chemical potential $(\mu_c^{\text{BLG}}(T))$ can be evaluated from Eqs. (B.11) & (B.15);

$$\frac{2mE_f^{\text{BLG}}}{\pi\hbar^2} = \frac{2m}{\pi\hbar^2} \left(\int_0^\infty dE \frac{1}{1+e^{(E^{\text{BLG}}-\mu_c^{\text{BLG}})/k_B T}} - \int_0^\infty dE \frac{1}{1+e^{(E^{\text{BLG}}+\mu_c^{\text{BLG}})/k_B T}} \right). \quad (\text{B.18})$$

Using the scaled parameter; $\frac{E^{\text{BLG}}}{E_f^{\text{BLG}}} = x$, $\frac{\mu_c^{\text{BLG}}}{E_f^{\text{BLG}}} = s$ and $\frac{T}{T_f} = y$, Eq.(B.18) can be written as

$$1 = \int_0^\infty dx \frac{1}{1+e^{(x-s)/y}} - \int_0^\infty dx \frac{1}{1+e^{(x+s)/y}} \quad (\text{B.19})$$

$$s = 1 \Rightarrow \mu = E_f \quad (\text{B.20})$$

Equation (B.20) shows that the chemical potential of BLG is temperature independent and very different from that of the MLG.

[III] Monolayer Gapped Graphene (MLLG)

The expression of chemical potential for MLGG can be defined same as that of MLG by introducing Eq. (B.14) into Eq. (B.15).