1 Electrons get their Bands and Gaps

As shown in the figure below, in the k-space of a 2D square lattice (lattice constant: a), denote the points $\Gamma : (k_x, k_y)$ =(0,0), X : (π/a, 0), and W : ($\frac{\pi}{a}$, $\frac{\pi}{a}$). The nearly free electron band-structure assumes no crystal potential, but a lattice.

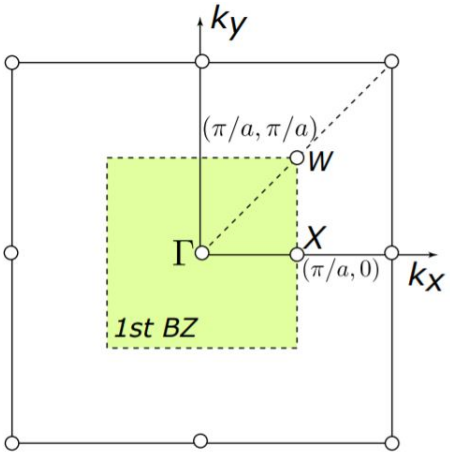

Figure 1: 2D reciprocal lattice

(a) Draw the nearly free-electron bandstructure from the BZ center in the $\Gamma - W$ direction slightly beyond the BZ edge. Identify the magnitude of k at the BZ edge, and express the energy in terms of $F = 2\pi^2\hbar^2/ma^2$. Include reciprocal lattice vectors smaller than $2 \times 2\pi/a$.

(b) Label each band with the reciprocal lattice vector it is associated with. Clearly point out the degeneracies of each band.

Consider now that the basis atoms produce a 2-D potential $V(x, y) = -4V_0 cos(\frac{2\pi x}{a}) cos(\frac{2\pi y}{a})$.

(c) Find the bandgap at the W point due to this potential. Be judicious in choosing the basis set.

(d) The lowest energy at the $\Gamma : (k_x, k_y) = (0, 0)$ point before the potential was turned on was $E_\Gamma(0, 0) = 0$ eV. Give an estimate of the change in this energy eigenvalue due to the periodic potential.

2 Exponential Approximation of the Fermi Function

When $E - E_f \gg$ KT, the Fermi function $f(E) = \frac{1}{e^{[(E-E_f)/KT]}+1}$ may be approximated by an exponential function. Similarly, when $E_f - E \gg$ KT, 1 - f(E) may be approximated by an exponential function. These conditions apply when the Fermi level lies within the bandgap, but away from its edges by an energy of a least several KT (at room temperature KT $\approx$ 0.026

eV whereas $E_g = 1.12$ eV in Si and 1.42 eV in GaAs). Using these approximations, which apply for both intrinsic (undoped) and doped semiconductors, show that

$$n = \int_{E_c}^{\infty} n(E)\mathrm{d}E, \quad p = \int_{-\infty}^{E_v} p(E)\mathrm{d}E,$$

where n and p are the concentration of electrons and holes (populations per unit volume), respectively. gives

$$n = N_c e^{-\frac{E_c - E_f}{KT}}$$
$$p = N_v e^{\frac{E_f - E_v}{KT}}$$
$$np = N_c N_v e^{-\frac{E_g}{KT}},$$

where $N_c = 2(\frac{2\pi m_c KT}{h^2})^{3/2}$ and $N_v = 2(\frac{2\pi m_v KT}{h^2})^{3/2}$. Verify that if E_f is closer to the conduction band and $m_v = m_c$, then $n > p$, whereas if it is closer to the valence band, then $p > n$.

3 Joint Density of States

Derive the joint density of states J_{cv} for one-dimensional and two-dimensional critical points.

4 Absorption coefficient for interband transitions

Assume an isotropic solid with band maxima and minima at $k = 0$. Show that the absorption coefficient for forbidden direct transitions is proportional to $(h\omega - \mathscr{E}_0)^{3/2}/h\omega$, where $\mathscr{E}_0$ is the direct band gap energy. Show that for indirect transitions from the valence band maximum to conduction band minima near the Brillouin zone boundary, the absorption coefficient is given by the equation:

$$\alpha \propto \int_0^{\hbar\omega \pm \hbar\omega_k - \mathscr{E}_G} (\hbar\omega \pm \hbar\omega_k - \mathscr{E}_G)^{3/2} \mathscr{E}^{1/2} \mathrm{d}\mathscr{E} \propto (\hbar\omega \pm \hbar\omega_k - \mathscr{E}_G)^3.$$

5 Graphene Density of States, Fermi-Dirac distribution

The electrons in the conduction band of graphene are free to move in 2-dimensions, forming a 2-dimensional electron gas (2DEG). The energy-momentum dispersion relationship for the 2DEG electrons in graphene is $E(k_x, k_y) = \upsilon_F \sqrt{k_x^2 + k_y^2}$, where υ_F is a parameter with dimensions of velocity. For graphene, it is $\upsilon_F = 10^8$ cm/s.

(a) Make a sketch of the energy as a function of the (k_x, k_y) points in the 2D k-space plane, and show that the dispersion results in a conical shape.

(b) Show that the density of states for these electrons is $g(E) = \frac{g_s g_\upsilon}{2\pi(\upsilon_F)^2}|E|$, where $g_s = 2$ is the spin degeneracy of each (k_x, k_y) state, and g_υ is the number of cones in the energy dispersion. For graphene, $g_\upsilon = 2$.

(c) Show that at thermal equilibrium, when the Fermi level is at $E_f = 0$, the number of conduction electrons per unit area in 2D graphene is $n_i = \frac{\pi}{6}(\frac{kT}{\hbar v_F})^2$. Make a plot of this density as a function of temperature for 0K $\leq$ T $\leq$ 500K. Explain why your plot sets the bar on the lowest possible density of carriers achievable in graphene at those temperatures.