ECE 4070: Exam 1 Solutions (By Farhan Rana)

Problem 1 (Benzene molecule) – 40 points

a) 6 (the number of orbitals and energy levels in LCAO is conserved)

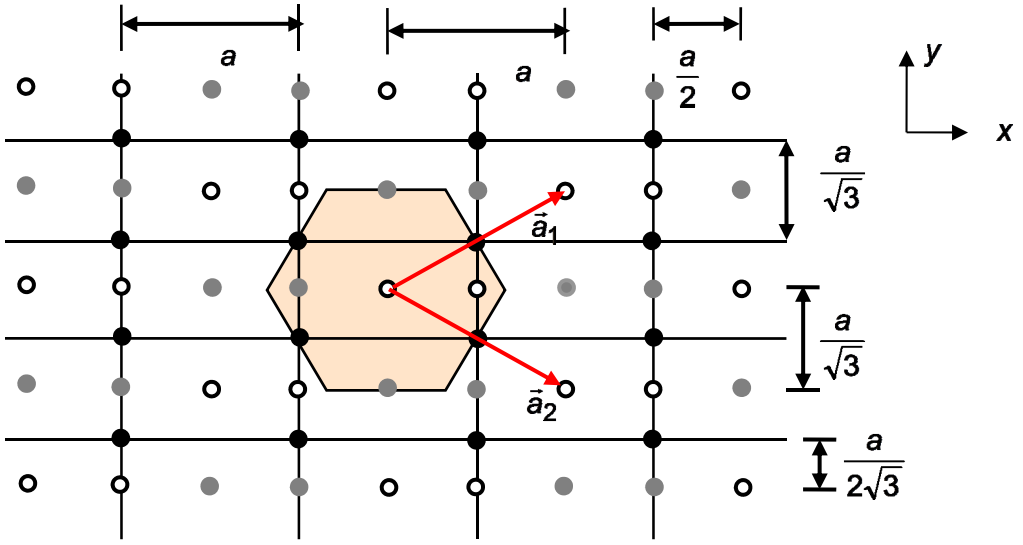
b) $$H = \begin{bmatrix} E_p & -V_{pp\pi} & & & & -V_{pp\pi} \\ -V_{pp\pi} & E_p & -V_{pp\pi} & & & \\ & -V_{pp\pi} & E_p & -V_{pp\pi} & & \\ & & -V_{pp\pi} & E_p & -V_{pp\pi} & \\ & & & -V_{pp\pi} & E_p & -V_{pp\pi} \\ -V_{pp\pi} & & & & -V_{pp\pi} & E_p \end{bmatrix}$$

c) For n=1,2,3,4 the equation for the coefficients is: $E_p c_n - V_{pp\pi}\left[c_{n-1} + c_{n+1}\right] = Ec_n$. Plugging in the given value of the coefficients one obtains: $E_p - 2V_{pp\pi}\cos(s) = E$. But for n=0, one gets: $E_p c_0 - V_{pp\pi}\left[c_5 + c_1\right] = Ec_0$ which, upon substitution of the given value of the coefficients yields: $E_p - V_{pp\pi}\left[e^{i5s} + e^{is}\right] = E$. This equation is the same as that obtained for n=1,2,3,4 if, and only if, $e^{i6s} = 1$. The condition $e^{i6s} = 1$ can also be understood from the intuitive argument that the wavefunction needs to be single valued after one complete rotation of the index "n". In other words, this condition implies the same periodic boundary condition that we had used earlier in the course. The condition $e^{i6s} = 1$ gives: $s = m\pi/3$, where m is an integer that goes from -2 to +3 (or from 0 to 5; any 6 consecutive integers would do without affecting the physical form of the wavefunction or the energy eigenvalues).

d) $E = E_p - 2V_{pp\pi}\cos(s)$, where $s = m\pi/3$, with $m = -2,-1,0,1,2,3$

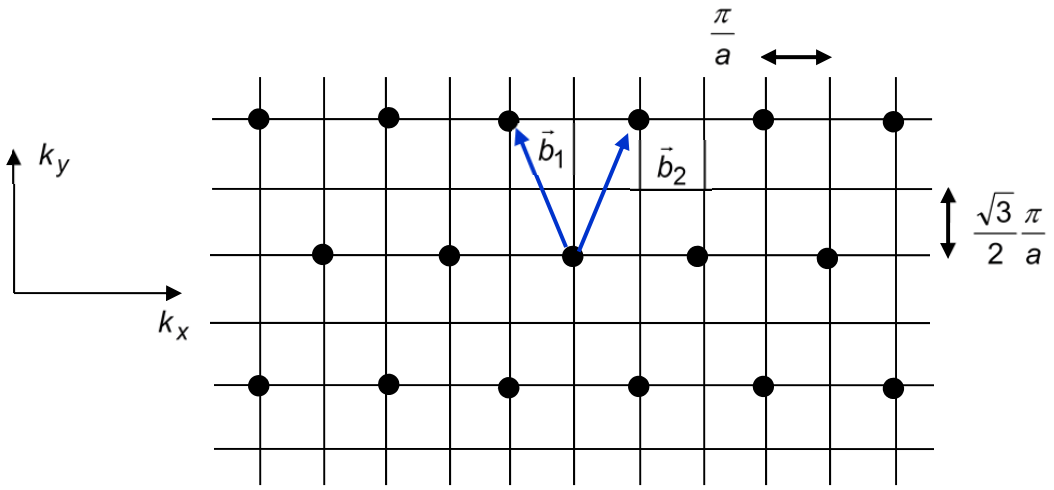
Problem 2 (2D lattice) – 30 points

a+b) $\vec{a}_1 = a\hat{x} + \frac{a}{\sqrt{3}}\hat{y}$ $\quad \vec{a}_2 = a\hat{x} - \frac{a}{\sqrt{3}}\hat{y}$. This a hexagonal lattice.



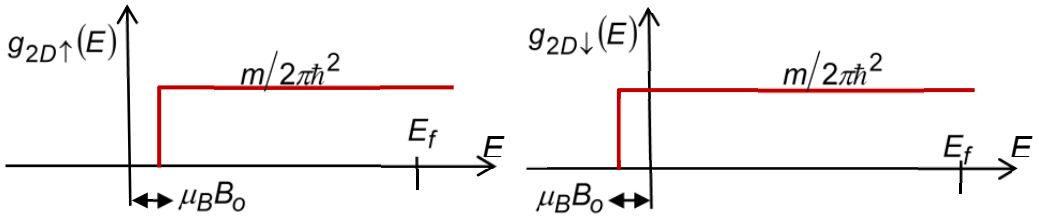
c) There are two A toms, two B atoms, and two C atoms in the Wigner Seitz Primitive cell.

d) $\vec{b}_1 = \frac{\pi}{a}\left[-\hat{x} + \sqrt{3}\,\hat{y}\right]$ $\qquad \vec{b}_1 = \frac{\pi}{a}\left[-\hat{x} - \sqrt{3}\,\hat{y}\right]$



Problem 3 (Misc) – 30 points

a) The lowest possible energy for spin-up electrons is $\mu_B B_o$ and for spin-down electrons it is $-\mu_B B_o$ .The spin-field coupling therefore just adds a constant term to the electron energy. The density of states for each type of electron is therefore sifted in energy and starts from a non-zero value as shown below.



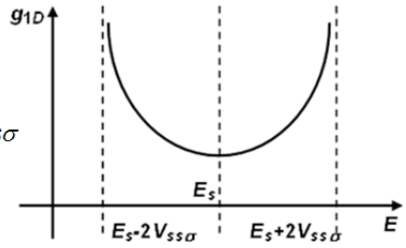
Since the 2D density of states for each type of electrons is independent of energy and since the temperature is near zero, the densities of spin-up and spin-down electrons are given by:

$$n_\uparrow = \frac{m}{2\pi\hbar^2}(E_f - \mu_B B_o) \qquad n_\downarrow = \frac{m}{2\pi\hbar^2}(E_f + \mu_B B_o) \qquad \Rightarrow n_\downarrow - n_\uparrow = \frac{m}{\pi\hbar^2}\mu_B B_o$$

b) $E(\vec{k}) = E_s - 2V_{ss\sigma}\cos(k_x a) \quad \Rightarrow \quad dE = 2V_{ss\sigma}\sin(k_x a)dk = \sqrt{4V_{ss\sigma}^2 - (E-E_s)^2}\,dk$

$$\Rightarrow \quad 2\times\int_{-\pi/a}^{+\pi/a}\frac{dk}{2\pi} = \frac{2}{\pi}\times\int_0^{+\pi/a}dk = \frac{2}{\pi}\times\int_{E_s-2V_{ss\sigma}}^{E_s+2V_{ss\sigma}}dE\,\frac{1}{\sqrt{4V_{ss\sigma}^2-(E-E_s)^2}}$$

$$\Rightarrow \quad g_{1D}(E) = \begin{cases} (2/\pi)\Big/\sqrt{4V_{ss\sigma}^2-(E-E_s)^2} & E_s - 2V_{ss\sigma} < E < E_s + 2V_{ss\sigma} \\ 0 & \text{Otherwise} \end{cases}$$



c) $E(\vec{k}) = \hbar v\sqrt{k_x^2+k_y^2} = \hbar v k \quad \Rightarrow \quad dE = \hbar v\,dk$

$$\Rightarrow \quad 2\times\iint\frac{d^2\vec{k}}{(2\pi)^2} = 2\times\int_0^\infty\frac{2\pi\,k\,dk}{(2\pi)^2} = \frac{1}{\pi}\times\int_0^\infty k\,dk = \frac{1}{\pi(\hbar v)^2}\times\int_0^\infty E\,dE \quad \Rightarrow \quad g_{2D}(E) = \frac{E}{\pi(\hbar v)^2} \qquad 0 \le E \le \infty$$