ECE 659, PRACTICE EXAM II
Actual Exam
Friday, Feb.21, 2014, FNY B124, 330-420PM

CLOSED BOOK

Useful relation $\left[h(\vec{k})\right] = \sum_m [H_{nm}]\, e^{+i\vec{k}.(\vec{r}_m-\vec{r}_n)}$

Actual Exam will have five questions.

The following questions have been chosen to stress what I consider the most important concepts / skills that you should be clear on.

2.1. Hydrogen atom wavefunctions (*QTAT, Ch.2*) **
2.2. Self-consistent field (*QTAT, Ch.3*) **
2.3. Dispersion relation for differential equation (Video L1.3, Tutorial 1.1)
2.4. Dispersion relation for 1D matrix equation (Video L1.3, Tutorial 1.1)
2.5. Dispersion relation for 2D lattice (Video L1.4, Tutorial 1.1)
2.6. Dispersion relation for 1D matrix equation with basis (Video L1.5)
2.7. Counting states for a discrete lattice (Tutorial 1.2,1.3) **
2.8. Graphene: Atomistic model to "effective mass" model
(Video L1.6, Tutorial 1.4)
2.9. Reciprocal lattice, Brillouin zone, counting valleys (*QTAT, Ch.5, 6*)
2.10. Subbands (*QTAT, Ch.6*)

** It may be instructive to try out MATLAB-based numerical examples, please see "MATLAB-based homework" posted on website.

Text: *Lecture 18, LNE*
(Lessons from Nanoelectronics), World Scientific (2012)

Reference: *Chapters 2-7, QTAT*
(Quantum Transport: Atom to Transistor), Cambridge (2005)

2.1.

(a) Show that the Schrodinger equation for a hydrogen atom

$$E\,\psi(\vec{r}) = \left(-\frac{\hbar^2}{2m}\nabla^2 \quad - \quad \frac{q^2}{4\pi\varepsilon_0 r}\right)\psi(\vec{r}) \tag{1a}$$

$$\nabla^2 \equiv \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\,\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right) \tag{1b}$$

is satisfied by a solution of the form $\psi(\vec{r}) = R(r)\,Y_\ell^m(\theta,\phi)$ provided

$$E\,R(r) = \left(-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) - \frac{q^2}{4\pi\varepsilon_0 r} + \frac{\hbar^2 l(l+1)}{2m r^2}\right)R(r) \tag{2a}$$

Note: $Y_\ell^m(\theta,\phi)$ are the spherical harmonics which satisfy the differential equation:

$$\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\,\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)Y_\ell^m \quad = \quad -\,\ell(\ell+1)\,Y_l^m \tag{2b}$$

SOLUTION:

Substituting $\psi(\vec{r}) = R(r)\,Y_\ell^m(\theta,\phi)$ into (1) and making use of (2b),

$$E\,R(r)Y_\ell^m(\theta,\phi) = \left(-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) - \frac{q^2}{4\pi\varepsilon_0 r} + \frac{\hbar^2 l(l+1)}{2m r^2}\right)R(r)Y_\ell^m(\theta,\phi)$$

Canceling $Y_\ell^m(\theta,\phi)$ we have (2a).

(b) Show that a solution of the form $R(r) = \dfrac{f(r)}{r}$ satisfies (2a) provided

$$E\,f(r) = \left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} - \frac{q^2}{4\pi\varepsilon_0 r} + \frac{\hbar^2\,\ell(\ell+1)}{2mr^2}\right)f(r) \tag{3}$$

SOLUTION:

We know that

$$\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right)\frac{f(r)}{r}= \left(\frac{d}{dr}+\frac{2}{r}\right)\frac{d}{dr}\frac{f(r)}{r}= \left(\frac{d}{dr}+\frac{2}{r}\right)\left(\frac{f'}{r}-\frac{f}{r^2}\right)$$

$$= \frac{f''}{r}-\frac{f'}{r^2}-\frac{f'}{r^2}+\frac{2f}{r^3}+\frac{2f'}{r^2}-\frac{2f}{r^3}= \frac{f''}{r}$$

Now substituting R(r) = f(r)/r in (2a), we have (3).

(c) We could solve (3) with ℓ=0 for the "s" levels, with ℓ=1 for the "p" levels with ℓ=2 for the "d" levels etc. But let us focus only on the first one (ℓ=0). Show that a solution of the form $f(r)= r\,e^{-r/a_0}$ satisfies (3) provided $a_0 = \dfrac{4\pi\,\varepsilon_0\,\hbar^2}{m\,q^2}$ and that the corresponding energy E is equal to $\dfrac{q^2}{8\pi\,\varepsilon_0\,a_0}$

SOLUTION: For 1s level, $\ell = 0$. Substituting $f(r)= re^{-r/a_0}$ into (3)

$$E\,re^{-r/a_0} = \left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}-\frac{q^2}{4\pi\varepsilon_0 r}\right)re^{-r/a_0}$$

$$= \left(-\frac{\hbar^2}{2ma_0}\frac{d^2}{d\rho^2}-\frac{q^2}{4\pi\varepsilon_0\rho}\right)\rho e^{-\rho} \quad , \quad \rho\equiv r/a_0$$

$$= \left(-\frac{\hbar^2}{2ma_0}\frac{d}{d\rho}\right)(1-\rho)e^{-\rho}-\frac{q^2}{4\pi\varepsilon_0}e^{-\rho}$$

$$= \frac{\hbar^2}{2ma_0}(2-\rho)e^{-\rho}-\frac{q^2}{4\pi\varepsilon_0}e^{-\rho}$$

$$E\,a_0\rho e^{-\rho} = \left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}-\frac{q^2}{4\pi\varepsilon_0 r}\right)re^{-r/a_0} = -\frac{\hbar^2}{2ma_0}\rho e^{-\rho}+\underbrace{\left(\frac{\hbar^2}{ma_0}-\frac{q^2}{4\pi\varepsilon_0}\right)}_{=0}e^{-\rho}$$

$$\frac{\hbar^2}{ma_0}=\frac{q^2}{4\pi\varepsilon_0} \quad\to\quad a_0=\frac{4\pi\varepsilon_0\hbar^2}{mq^2}$$

$$E = -\frac{\hbar^2}{2ma_0^2}= -\frac{q^2}{8\pi\varepsilon_0 a_0}$$

2.2. Self-consistent field

(a) Suppose we write the Schrodinger equation for a helium atom as

(atomic number Z=2)

$$E\,\psi(\vec{r}) = \left(-\frac{\hbar^2}{2m}\nabla^2 - \frac{Zq^2}{4\pi\varepsilon_0 r}\right)\psi(\vec{r}) \qquad (4)$$

Proceeding as in Problem 2.1, with ℓ=0 for the "s" levels , we obtain the radial equation

$$E\,f(r) = \left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} - \frac{Z\,q^2}{4\pi\varepsilon_0 r}\right)f(r)$$

Assuming a solution of the form $f(r) = \; r\,e^{-r/a}$ find 'a' and the corresponding energy E.

SOLUTION:

Proceeding as in Problem 2.1c, we now obtain

$$\frac{\hbar^2}{ma} = \frac{Z\,q^2}{4\pi\varepsilon_0} \quad \rightarrow \quad a = \frac{4\pi\varepsilon_0\hbar^2}{Z\,mq^2} = \frac{a_0}{Z}$$

$$E = \; -\frac{\hbar^2}{2ma^2} = \; -\frac{Z\,q^2}{8\pi\varepsilon_0 a}$$

(b) Based on Part (a), what would you predict the energy of an 1s level in Helium to be, given that the energy of an 1s level in Hydrogen is -13.6 eV.
Is this result correct ? Explain.

SOLUTION:

Since Z=2 for Helium, the energy should be 4 times that of Hydrogen, or -53.4 eV.

This result is not correct because it does not include the self-consistent field due to the other electron in Helium. The measured ionization potential for Helium is ~ -25 eV, which is about 30eV higher, due to the repulsive potential from the other electron.

However, the second ionization potential needed to turn He^{+} into He^{++} is approximately ~- -53 eV.

2.3. Consider a pair of coupled differential equations of the form ($\vec{p} \equiv \; -i\hbar\vec{\nabla}$) :

$$E\begin{Bmatrix}\psi(x,y)\\ \varphi(x,y)\end{Bmatrix} = \begin{bmatrix}\varepsilon & v_0(p_x - ip_y)\\ v_0(p_x + ip_y) & -\varepsilon\end{bmatrix}\begin{Bmatrix}\psi(x,y)\\ \varphi(x,y)\end{Bmatrix}$$

Find the dispersion relation $E(k_x, k_y)$? What are the eigenfunctions ?

SOLUTION:

Solutions can be written in the form $\begin{Bmatrix}\psi(x,y)\\ \varphi(x,y)\end{Bmatrix} = \begin{Bmatrix}\psi_0\\ \varphi_0\end{Bmatrix} e^{i(k_x x + k_y y)}$

Substituting into original differential equation

$$E\begin{Bmatrix}\psi_0\\ \varphi_0\end{Bmatrix} = \begin{bmatrix}\varepsilon & -i\hbar v_0(ik_x + k_y)\\ -i\hbar v_0(ik_x - k_y) & -\varepsilon\end{bmatrix}\begin{Bmatrix}\psi_0\\ \varphi_0\end{Bmatrix}$$

so that the eigenvalues are given by

$$E \;=\; \pm\sqrt{\varepsilon^2 + \hbar^2 v_0^2 (k_x^2 + k_y^2)}$$

and the eigenvectors can be written as (please check)

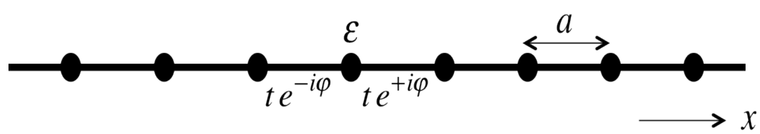
$$\begin{Bmatrix}c\\ s\end{Bmatrix} \;\; and \;\; \begin{Bmatrix}-s^*\\ c^*\end{Bmatrix}$$

$$c \equiv \; \cos\frac{\theta}{2}\, e^{-i\varphi/2} \;, \quad s \equiv \; \sin\frac{\theta}{2}\, e^{+i\varphi/2} \;,$$

where

$$\theta \equiv \tan^{-1}\frac{\hbar v_0 \sqrt{k_x^2 + k_y^2}}{\varepsilon} \;\;, \;\; \varphi \equiv \tan^{-1}\frac{k_y}{k_x}$$

2.4. How would you choose the parameters ε, t *and* φ for a 1D lattice described by



$$E\psi_n \;=\; t\,e^{-i\varphi}\,\psi_{n-1} + \varepsilon\psi_n + t\,e^{+i\varphi}\,\psi_{n+1}$$

so that the dispersion relation matches that of the differential equation

$$E\psi \;=\; \frac{(p+qA)^2}{2m}\,\psi\,, \qquad p \equiv -i\hbar\frac{\partial}{\partial x}\;,\; A:\text{constant}$$

for small values of ka.

SOLUTION:

Dispersion relation for differential equation obtained by inserting $\psi \sim e^{+ikx}$:

$$E \;=\; \frac{(\hbar k + qA)^2}{2m}$$

Dispersion relation for matrix equation obtained by inserting $\psi \sim e^{+ikna}$:

$$E \;=\; t\,e^{-i\varphi}\,e^{-ika} + \varepsilon + t\,e^{+i\varphi}\,e^{+ika} \;=\; \varepsilon + 2t\cos(ka+\varphi)$$

Using Taylor expansion for small ka,

$$E \;\approx\; \varepsilon + 2t\left(1 - \frac{(ka+\varphi)^2}{2}\right) \;=\; (\varepsilon+2t) - ta^2\left(k+\frac{\varphi}{a}\right)^2$$

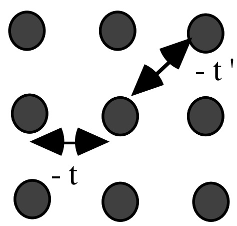
Comparing with $\quad E \;=\; \dfrac{\hbar^2}{2m}\left(k+\dfrac{qA}{\hbar}\right)^2$

we have $\quad \varepsilon + 2t = 0\,,\quad t = -\dfrac{\hbar^2}{2ma^2}\,,\quad \varphi = \dfrac{qAa}{\hbar}$

2.5. The $E(k_x,k_y)$ relation for some solids is often written in the form

$$E = E_0 - 2V\,(\cos k_x a + \cos k_y a + 2\alpha \cos k_x a \cos k_y a)$$

where α is a dimensionless number. How would you choose the nearest neighbor and next nearest neighbor overlap matrix elements in a square lattice of side 'a' so as to correspond to this dispersion relation ?



Nearest neighbor overlap : - t

Next nearest neighbor overlap : - t'

SOLUTION:

$$E = \varepsilon - t\left(e^{ik_x a} + e^{-ik_x a} + e^{ik_y a} + e^{-ik_y a}\right)$$
$$-t'\left(e^{i(k_x+k_y)a} + e^{i(k_x-k_y)a} + e^{i(-k_x+k_y)a} + e^{i(-k_x-k_y)a}\right)$$

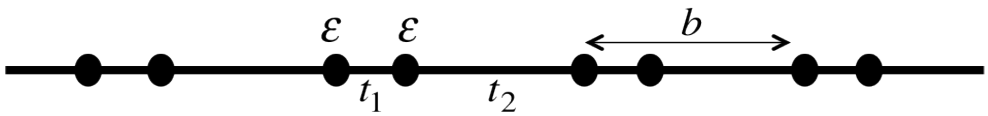
$$= \varepsilon - 2t\left(\cos k_x a + \cos k_y a\right) - 2t'\left(e^{ik_x a}\cos k_y a + e^{-ik_x a}\cos k_y a\right)$$

$$= \varepsilon - 2t\left(\cos k_x a + \cos k_y a\right) - 4t'\cos k_y a \cos k_y a$$

Comparing,

$$\varepsilon = E_0\,, \quad t = V\,, \quad t' = V\alpha$$

2.6. Consider a 1D tight-binding model with a nearest neighbor coupling that alternates between two values t_1 and t_2 as shown.



Find the dispersion relation E(k) and eigenvectors for a given value of k.

SOLUTION:

$$h(k) = \begin{bmatrix} 0 & t_2 \\ 0 & 0 \end{bmatrix} e^{-ikb} + \begin{bmatrix} \varepsilon & t_1 \\ t_1 & \varepsilon \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ t_2 & 0 \end{bmatrix} e^{+ikb} \quad = \begin{bmatrix} \varepsilon & t_1 + t_2 e^{-ikb} \\ t_1 + t_2 e^{+ikb} & \varepsilon \end{bmatrix}$$

$$\begin{aligned} E(k) = & \ \varepsilon \pm \sqrt{(t_1 + t_2 e^{+ikb})\,(t_1 + t_2 e^{-ikb})} \\ = & \ \varepsilon \pm \sqrt{t_1^2 + t_2^2 + 2 t_1 t_2 \cos kb} \end{aligned}$$

Eigenvectors can be written as (please check)

$$\frac{1}{\sqrt{2}} \begin{Bmatrix} 1 \\ e^{+i\varphi} \end{Bmatrix} \ \textit{and} \ \frac{1}{\sqrt{2}} \begin{Bmatrix} -1 \\ e^{+i\varphi} \end{Bmatrix}, \quad \varphi \equiv \tan^{-1} \frac{t_2 \sin kb}{t_1 + t_2 \cos kb}$$

2.7. Use the principles of bandtructure to write down the eigenvalues of these 6x6 matrices

(a)

$$\begin{bmatrix} \varepsilon & t & 0 & 0 & 0 & t \\ t & \varepsilon & t & 0 & 0 & 0 \\ 0 & t & \varepsilon & t & 0 & 0 \\ 0 & 0 & t & \varepsilon & t & 0 \\ 0 & 0 & 0 & t & \varepsilon & t \\ t & 0 & 0 & 0 & t & \varepsilon \end{bmatrix}$$

(b)

$$\begin{bmatrix} \varepsilon & t & 0 & 0 & 0 & 0 \\ t & \varepsilon & t & 0 & 0 & 0 \\ 0 & t & \varepsilon & t & 0 & 0 \\ 0 & 0 & t & \varepsilon & t & 0 \\ 0 & 0 & 0 & t & \varepsilon & t \\ 0 & 0 & 0 & 0 & t & \varepsilon \end{bmatrix}$$

(c)

$$\begin{bmatrix} \varepsilon & t_1 & 0 & 0 & 0 & t_2 \\ t_1 & \varepsilon & t_2 & 0 & 0 & 0 \\ 0 & t_2 & \varepsilon & t_1 & 0 & 0 \\ 0 & 0 & t_1 & \varepsilon & t_2 & 0 \\ 0 & 0 & 0 & t_2 & \varepsilon & t_1 \\ t_2 & 0 & 0 & 0 & t_1 & \varepsilon \end{bmatrix}$$

SOLUTION:

(a) $\varepsilon + 2t\cos[-3 \quad -2 \quad -1 \quad 0 \quad +1 \quad +2].*2\pi/6$

-2.0000 -1.0000 -1.0000 1.0000 1.0000 2.0000

(b) $\varepsilon + 2t\cos[1 \quad 2 \quad 3 \quad 4 \quad 5 \quad 6].*\pi/7$

-1.8019 -1.2470 -0.4450 0.4450 1.2470 1.8019

(c) $\varepsilon \pm \sqrt{t_1^2 + t_2^2 + 2t_1 t_2 \cos[-1 \quad 0 \quad +1].*2\pi/3}$

-2.0000 -1.3229 -1.3229 1.3229 1.3229 2.0000

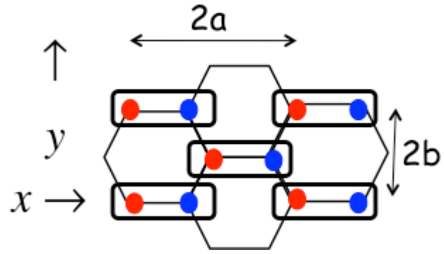
2.8. Graphene has an atomic structure as shown. Assume a nearest neighbor tight-binding model with

$$\vec{a}_1 = a\hat{x} + b\hat{y}$$
$$\vec{a}_2 = a\hat{x} - b\hat{y}$$

$$H_{n,n} = \varepsilon$$

$H_{n,m} = t$ if n, m are neighboring atoms

$H_{n,m} = 0$ if n, m are NOT nearest neighbors



Show that $E(k_x, k_y)$ can be written as

$$E(k_x, k_y) = \varepsilon \pm at\sqrt{\beta_x^2 + \beta_y^2}$$

where

$$\beta_x = k_x - k_{x0}, \quad \beta_y = k_y - k_{y0} \quad , \qquad k_{x0} = 0, k_{y0} = \frac{2\pi}{3b}$$

SOLUTION:

$$h(k_x, k_y) = e^{-i\vec{k}.\vec{a}_2}\begin{bmatrix} 0 & t \\ 0 & 0 \end{bmatrix} + e^{-i\vec{k}.\vec{a}_1}\begin{bmatrix} 0 & t \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} \varepsilon & t \\ t & \varepsilon \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ t & 0 \end{bmatrix} e^{+i\vec{k}.\vec{a}_1} + \begin{bmatrix} 0 & 0 \\ t & 0 \end{bmatrix} e^{+i\vec{k}.\vec{a}_2}$$

$$= \begin{bmatrix} \varepsilon & h_0^* \\ h_0 & \varepsilon \end{bmatrix},$$

where $h_0 \equiv t + te^{+i\vec{k}.\vec{a}_1} + te^{+i\vec{k}.\vec{a}_2} = t(1 + 2e^{ik_x a}\cos k_y b)$

The two branches of the dispersion relation are given by the eigenvalues of $h(k_x, k_y)$:

$$E(k_x, k_y) = \varepsilon \pm \left| h_0(k_x, k_y) \right|$$

Expand h_0 around one of the valleys like (k_{x0}, k_{y0}) where $h_0 = 0$.

$$\left(\frac{\partial h_0}{\partial k_x}\right)_{\substack{k_x=0 \\ k_y=2\pi/3b}} = \left(2t\, ia\, e^{ik_x a}\cos k_y b\right)_{\substack{k_x=0 \\ k_y=2\pi/3b}} = -iat$$

$$\left(\frac{\partial h_0}{\partial k_y}\right)_{\substack{k_x=0 \\ k_y=2\pi/3b}} = \left(-2t\, b\, e^{ik_x a}\sin k_y b\right)_{\substack{k_x=0 \\ k_y=2\pi/3b}} = -\sqrt{3}\, tb = -ta$$

Hence $h_0(k_x, k_y) \approx \; -iat\,\beta_x - ta\,\beta_y \;=\; -iat(\beta_x + i\,\beta_y)$

$$\left|h_0(k_x, k_y)\right| \;=\; at\sqrt{\beta_x^2 + \beta_y^2}$$

so that
$$E(k_x, k_y) = \; \varepsilon \pm at\sqrt{\beta_x^2 + \beta_y^2}$$

2.9. How many conduction valleys does graphene have? Explain.

Conduction valleys occur around the zeros of h_0 (k_x , k_y) given by

$$k_{x0} = 0, k_{y0} = \pm\frac{2\pi}{3b}$$

and $\quad k_{x0} = \pm\frac{\pi}{a}, k_{y0} = \pm\frac{\pi}{3b}$

The number of valleys depends on how many are contained within a Brillouin zone. To construct the Brillouin zone, first step is to find the reciprocal lattice vectors from the real space lattice vectors:

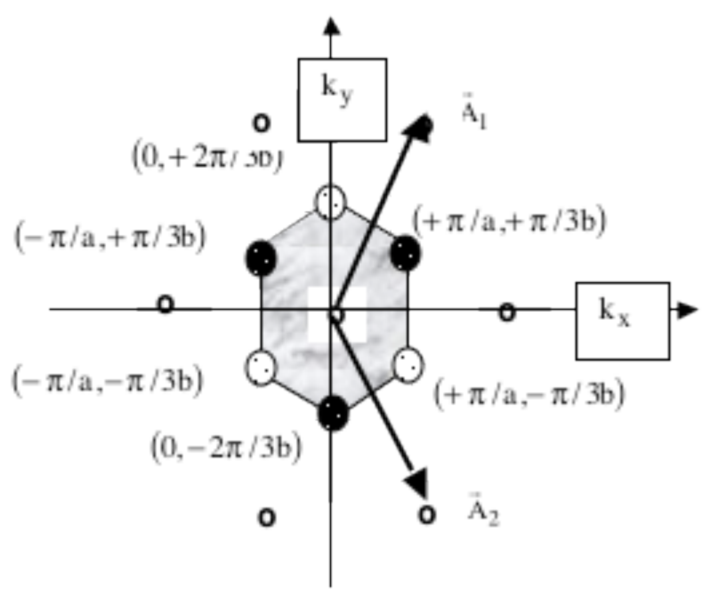
$$\vec{A}_1 = \frac{2\pi\,(\vec{a}_2 \text{ x } \vec{a}_3)}{\vec{a}_1 \cdot (\vec{a}_2 \text{ x } \vec{a}_3)}\;, \qquad \vec{A}_2 = \frac{2\pi\,(\vec{a}_3 \text{ x } \vec{a}_1)}{\vec{a}_2 \cdot (\vec{a}_3 \text{ x } \vec{a}_1)}$$

Since $\vec{a}_1 = \hat{x}\,a + \hat{y}\,b$, $\vec{a}_2 = \hat{x}\,a - \hat{y}\,b$, $\vec{a}_3 = \hat{z}\,c$, we have

$$\vec{A}_1 = \frac{2\pi\,(\vec{a}_2 \text{ x } \hat{z})}{\vec{a}_1 \cdot (\vec{a}_2 \text{ x } \hat{z})} \;=\; \hat{x}\left(\frac{\pi}{a}\right) + \hat{y}\left(\frac{\pi}{b}\right)$$

$$\vec{A}_2 = \frac{2\pi\,(\hat{z} \text{ x } \vec{a}_1)}{\vec{a}_2 \cdot (\hat{z} \text{ x } \vec{a}_1)} \;=\; \hat{x}\left(\frac{\pi}{a}\right) - \hat{y}\left(\frac{\pi}{b}\right)$$

Using these basis vectors we can construct the reciprocal lattice shown. The Brillouin zone is then obtained by drawing the perpendicular bisectors of the lines joining the origin (0,0) to the neighboring points on the reciprocal lattice.



Note that the valleys occur st the corners of the Brillouin zone so that only one-thirs of each valley is contained within a Brillouin zone. Hence the total number of valleys = 6 x (1/3) = 2.

2.10. (a) A sheet of graphene having a dispersion relation

$$E(k_x, k_y) = \quad \varepsilon \pm at\sqrt{\beta_x^2 + \beta_y^2}$$

where $\qquad \beta_x = k_x - k_{x0}, \quad \beta_y = k_y - k_{y0} \quad , \qquad k_{x0} = 0, k_{y0} = \dfrac{2\pi}{3b}$

is rolled up to form a nanotube with a circumferential vector along the x-direction: $\vec{c} = \hat{x}\, 2a\, m$, m being an integer. What is the dispersion relation $E_\nu(k_y)$ for subband ν. Is there a subband ν that has zero gap between the '+' and '-' branches?

SOLUTION: Periodic boundary condition along circumference:

$$\vec{k}.\vec{c} \quad = \quad 2\pi\nu \quad \rightarrow \quad k_x = \frac{2\pi\nu}{2ma}$$

$$E_\nu(k_y) = \quad \varepsilon \pm at\sqrt{\left(\nu\frac{\pi}{ma}\right)^2 + \beta_y^2} \;\; , \;\; \beta_y \equiv k_y - \frac{2\pi}{3b}$$

Subband with $\nu = 0$ has zero gap.

(b) A sheet of graphene is rolled up to form a nanotube with a circumferential vector along the y-direction: $\vec{c} = \hat{y}\, 2b\, m$, m being an integer. What is the dispersion relation $E_\nu(k_x)$ for subband ν. Is there a subband ν that has zero gap between the '+' and '-' branches?

SOLUTION: Periodic boundary condition along circumference:

$$\vec{k}.\vec{c} \quad = \quad 2\pi\nu \quad \rightarrow \quad k_y = \frac{2\pi\nu}{2mb}$$

$$E_\nu(k_y) = \quad \varepsilon \pm at\sqrt{k_x^2 \; + \left(\nu\frac{\pi}{mb} - \frac{2\pi}{3b}\right)^2}$$

Subband with $\nu = 2m/3$ has zero gap, only possible if m is a multiple of 3.