ECE 659, EXAM II

Friday, Feb.20, 2014, EE117, 230-320PM

NAME : SOLUTION

CLOSED BOOK

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

All five questions carry equal weight

Please show all work.
No credit for just writing down the answer, even if correct.

2.1. Consider the radial Schrodinger equation for an s-level in a helium atom (atomic number Z=2)

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

Assuming a solution of the form $f(r) = \; r\,e^{-r/a}$ obtain expressions for 'a' and the corresponding energy E in terms of the parameters appearing in (A).

SOLUTION:

Substituting $f(r) = \; re^{-r/a}$ into (A)

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

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

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

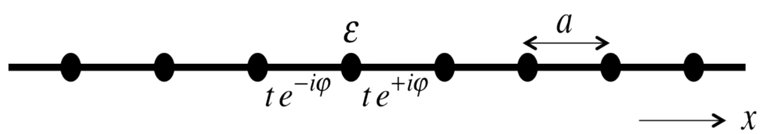
$$= \frac{\hbar^2}{2ma}(2-\rho)e^{-\rho} - \frac{q^2}{4\pi\varepsilon_0} e^{-\rho}$$

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

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

$$E = -\frac{\hbar^2}{2ma^2} = -\frac{Zq^2}{8\pi\varepsilon_0 a} = -\frac{Z^2 q^2}{8\pi\varepsilon_0 a_0}$$

2.2. How would you choose the parameters $\varepsilon, t \text{ and } \varphi$ 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 $\psi \sim e^{+ikna}$:

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

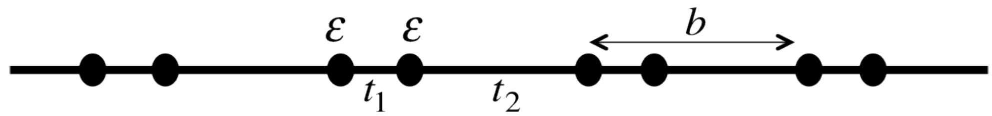
Using Taylor expansion for small ka,

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

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

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

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



The dispersion relation E(k) is given by

$$E(k) = \varepsilon \pm \sqrt{t_1^2 + t_2^2 + 2t_1 t_2 \cos kb}$$

Use this result to write down the eigenvalues of the (6x6) matrix, assuming $\varepsilon = 0\,, t_1 = 2\,, t_2 = 1$

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

SOLUTION:

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

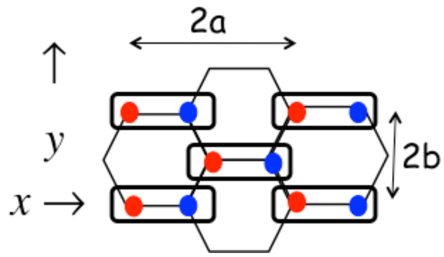
$$= \varepsilon \pm \sqrt{t_1^2 + t_2^2 + 2t_1 t_2 * [-1/2 \quad 1 \quad -1/2]}$$

$$= \pm\sqrt{5 + 4*[-1/2 \quad 1 \quad -1/2]}$$

$$= \pm\sqrt{3}\,, \pm 3\,, \pm\sqrt{3}$$

2.4. Graphene has an atomic structure as shown.

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



(a) Obtain the basis vectors for the reciprocal lattice.
(b) Draw the reciprocal lattice and show the first Brillouin zone.

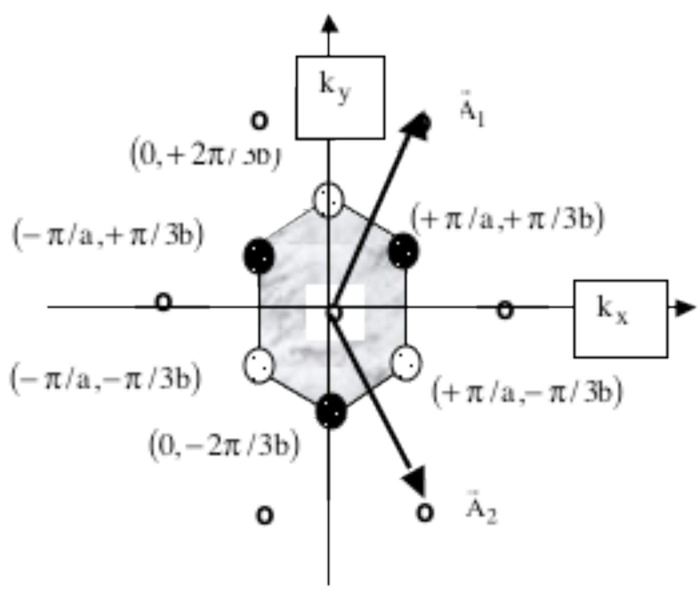
SOLUTION:

(a) 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

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

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

(b) 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.



2.5. A sheet of graphene having a dispersion relation

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

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

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:

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

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

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