Phy 240A | HW 4 Solutions

1. (a) $H_{11} = \varepsilon_1 + t_x\left(e^{ik_xa} + e^{-ik_xa}\right) + t_y\left(e^{ik_yb} + e^{-ik_yb}\right)$

$= \varepsilon_1 + \frac{1}{4}\cos k_x a + \cos k_y b \qquad \left(t_x = \frac{1}{8},\ t_y = \frac{1}{2}\right)$

$H_{22} = \varepsilon_2 + \cos k_y b$

$H_{12} = t\left(1 + e^{-ik_yb}\right)$

$= 1 + e^{-ik_yb} \qquad (t = 1)$

$H_{21} = H_{12}^\dagger$

$$\therefore H = \begin{bmatrix} \varepsilon_1 + \frac{1}{4}\cos k_x a + \cos k_y b & 1 + e^{-ik_yb} \\ 1 + e^{ik_yb} & \varepsilon_2 + \cos k_y b \end{bmatrix}$$

(b)

$$\begin{vmatrix} H_{11} - E & H_{12} \\ H_{21} & H_{22} - E \end{vmatrix} = 0$$

$\left(\varepsilon_1 + \frac{1}{4}\cos k_x a + \cos k_y b - E\right)\left(\varepsilon_2 + \cos k_y b - E\right) - \left(2 + 2\cos k_y b\right) = 0$

$E^2 + \varepsilon_1\varepsilon_2 + \varepsilon_1\cos k_y b - E\varepsilon_1 + \frac{1}{4}\varepsilon_2\cos k_x a + \frac{1}{4}\cos k_x a\cos k_y b - \frac{1}{4}E\cos k_x a$

$\quad + \varepsilon_2\cos k_y b + \cos^2 k_y b - E\cos k_y b - \varepsilon_2 E - E\cos k_y b - 2 - 2\cos k_y b = 0$

$E^2 + E\left(-\varepsilon_1 - \varepsilon_2 - \frac{1}{4}\cos k_x a - 2\cos k_y b\right) + \varepsilon_1\varepsilon_2 - 2 + \cos k_y b\left(\varepsilon_1 + \varepsilon_2 - 2 + \cos k_y b\right)$

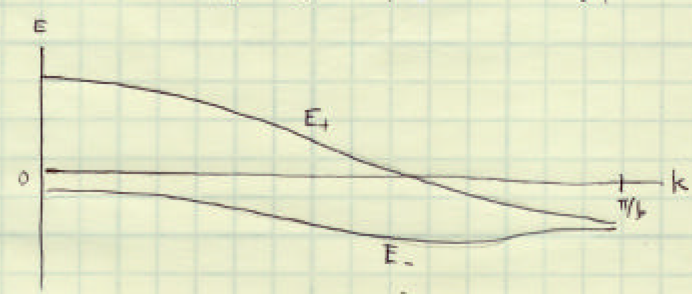
$\qquad + \frac{1}{4}\varepsilon_2\cos k_x a + \frac{1}{4}\cos k_x a\cos k_y b = 0$

Along the k_y axis, $k_x = 0$.

(i) For $\varepsilon_1 = \varepsilon_2 = 0$,

$E^2 + E\left(-\frac{1}{4} - 2\cos k_y b\right) + \cos^2 k_y b - \frac{7}{4}\cos k_y b - 2 = 0$

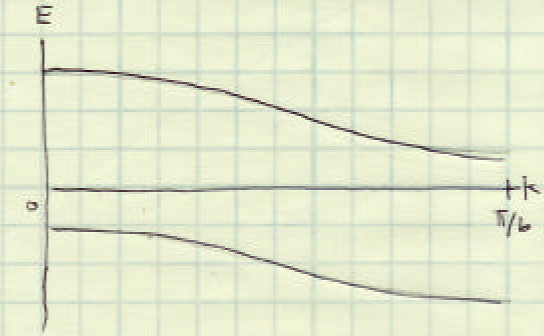
So $E = \cos k_y b + \frac{1}{8} \pm \sqrt{2\cos k_y b + \frac{129}{64}}$



(ii) For $\varepsilon_1 = 4$ & $\varepsilon_2 = -4$,

$$E^2 + E\left(-\frac{1}{4} - 2\cos k_y b\right) + \cos^2 k_y b - \frac{7}{4}\cos k_y b - 19 = 0$$

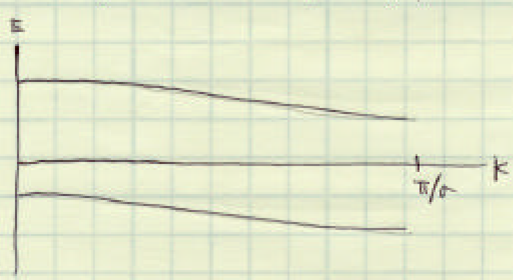
So $E = \cos k_y b + \frac{1}{8} \pm \sqrt{2\cos k_y b + \frac{1}{64} + 19}$



(c) $\varepsilon_1 = \varepsilon_2 = 0$; along k_x $(k_y = 0)$

$$E^2 - \left(2 + \frac{1}{4}\cos k_x a\right) + \frac{1}{4}\cos k_x a - 3 = 0$$

So $E = \frac{1}{8}\cos k_x a + 1 \pm \sqrt{4 + \frac{1}{64}\cos^2 k_x a}$



2. Free electrons in 2D

The DOS is

$$D(\varepsilon) = L^{-2} \sum_{\vec{k},\sigma} \delta(\varepsilon - \varepsilon(\vec{k}))$$

$$= 2L^{-2} \sum_{\vec{k}} \delta[\varepsilon - \varepsilon(\vec{k})]$$

$$\xrightarrow{L\to\infty} \int \frac{d\vec{k}}{4\pi^2} \delta[\varepsilon - \varepsilon(\vec{k})] \qquad \left(\because \Delta\vec{k} = \left(\frac{2\pi}{L}\right)^{\alpha} \text{ in } \alpha \text{ dimension}\right)$$

$$= \frac{1}{4\pi^2} \int 2\pi k\, dk\, \delta[\varepsilon - \varepsilon(\vec{k})]$$

$$k = \frac{\sqrt{2m\,\varepsilon(\vec{k})}}{\hbar}, \quad dk = \frac{\sqrt{2m}}{\hbar} \cdot \frac{1}{2}[\varepsilon(\vec{k})]^{-1/2}$$

So

$$D(\varepsilon) = \frac{1}{\pi} \int \frac{2m}{\hbar^2} \cdot \frac{1}{2} \delta[\varepsilon - \varepsilon(\vec{k})]$$

$$= \frac{m}{\pi\hbar^2}$$

In atomic units, $m = \hbar = 1$. So

$D(\varepsilon) = \frac{1}{\pi}$ (unitless)