PHYS 563 HW # 6

Wen-Hua Wu
(Wenhua / Wen Hua / Albert)
S01470274
aw106@rice.edu

Problem 1

By A&M (10.28) & (10.29),

we have

$$\phi_n(\vec{r}-\vec{R}) = \frac{1}{V_0}\int d\vec{k}\, e^{-i\vec{R}\cdot\vec{k}}\, \psi_{n\vec{k}}(\vec{r})$$

$$\therefore \int \phi_n^*(\vec{r}-\vec{R})\,\phi_m(\vec{r}-\vec{R'})\,d\vec{r} := \Phi_{mn;R\vec{R'}}$$

$$= \frac{1}{|V_0|^2}\int d\vec{k}\int d\vec{k'}\int d\vec{r}\, e^{i(\vec{R}\cdot\vec{k}-\vec{R'}\cdot\vec{k'})}\, \psi_{n\vec{k}}^*(\vec{r})\,\psi_{m\vec{k'}}(\vec{r})$$

We know that

$$\int d\vec{r}\, \psi_{n\vec{k}}^*(\vec{r})\psi_{m\vec{k'}}(\vec{r}) = \delta_{mn}\,\delta_{\vec{k}\vec{k'}}$$

$\because$ Each bloch function is an eigenfunction of the total Hamiltonian.

$$\therefore \Phi_{mn;R\vec{R'}} = \frac{\delta_{mn}}{|V_0|^2}\int d\vec{k}\int d\vec{k'}\, e^{i(\vec{R}\cdot\vec{k}-\vec{R'}\cdot\vec{k'})}\,\delta_{\vec{k}\vec{k'}}$$

$$= \frac{\delta_{mn}}{|V_0|^2}\int d\vec{k}\, e^{i(\vec{R}-\vec{R'})\cdot\vec{k}} = \frac{N\,\delta_{mn}}{|V_0|^2}\,\delta_{\vec{R}-\vec{R'}=0}$$

(by F.4)

$$\propto \delta_{mn}\,\delta_{\vec{R}\vec{R'}} \quad \vec{R}=\vec{R'}$$

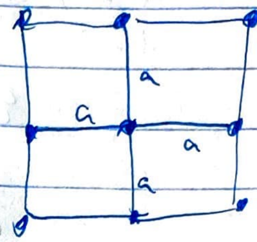
When $m=n$, we can see that

$$\int |\phi(\vec{r}-\vec{R})|^2 = 1 = \int |\phi(\vec{r})|^2$$

Problem 2.

(a)

Following A&M (10.19),



where $E_s = E_{atom} = 2E_0$

$\beta \approx 0$

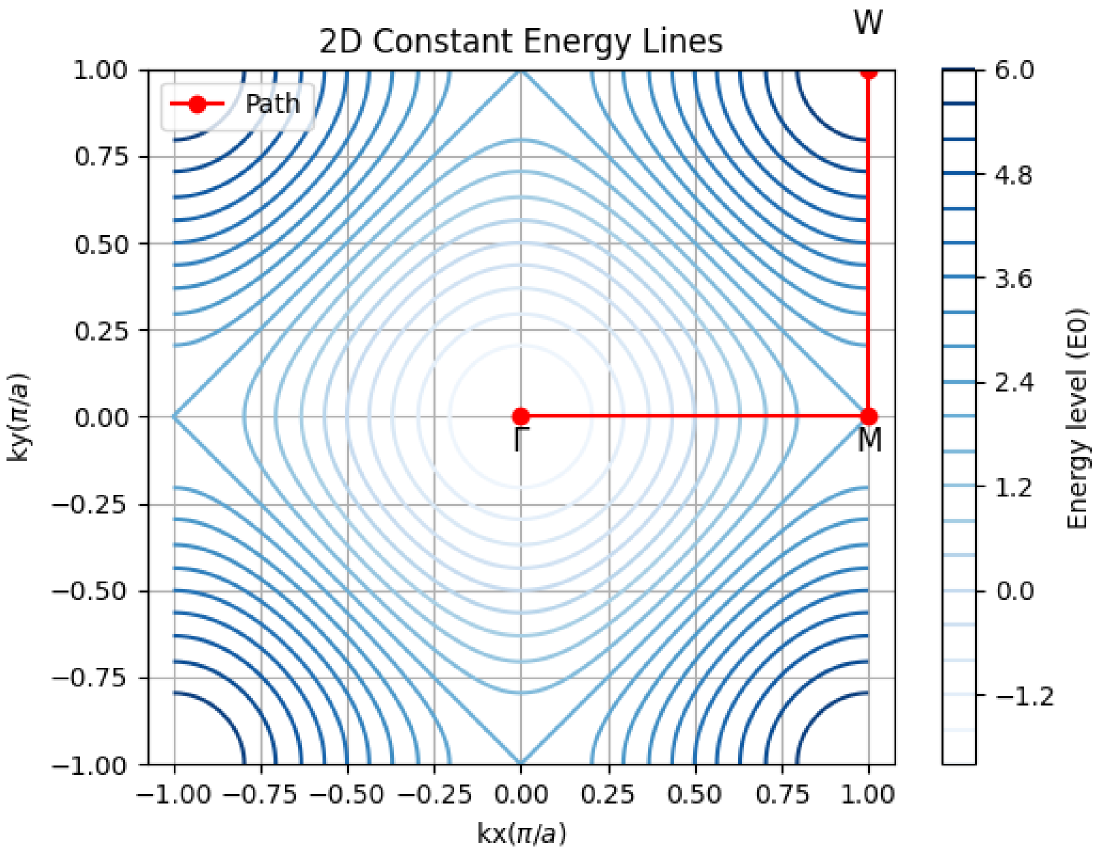
$\gamma(\vec{R}) = -t = E_0$ (for n.n.)

$$\varepsilon(\vec{k}) = E_s - \beta - \sum_{n.n.} \gamma(\vec{R}) \cos(\vec{k}\cdot\vec{R})$$

$$= 2E_0 - 2E_0 \left[\cos(k_x a) + \cos(k_y a)\right]$$

2(b)

Below is the 1st Brillioun Zone with some constant energy lines



(c) For a constant energy line

$\mathcal{E}(\vec{k}) = \mathcal{E}_0$, the implicit derivative of

$\frac{d k_y(k_x, \mathcal{E})}{d k_x}$ is

$$d\mathcal{E} = \frac{\partial \mathcal{E}(\vec{k})}{\partial k_x} dk_x + \frac{\partial \mathcal{E}(\vec{k})}{\partial k_y} dk_y = 0$$

$$\Rightarrow \frac{dk_y}{dk_x} = - \frac{\frac{\partial \mathcal{E}(\vec{k})}{\partial k_x}}{\frac{\partial \mathcal{E}(\vec{k})}{\partial k_y}} = \frac{-\sin(k_x a)}{\sin(k_y a)}$$

At $k_x = \pm \frac{\pi}{a}$, $\frac{dk_y}{dk_x} = 0$

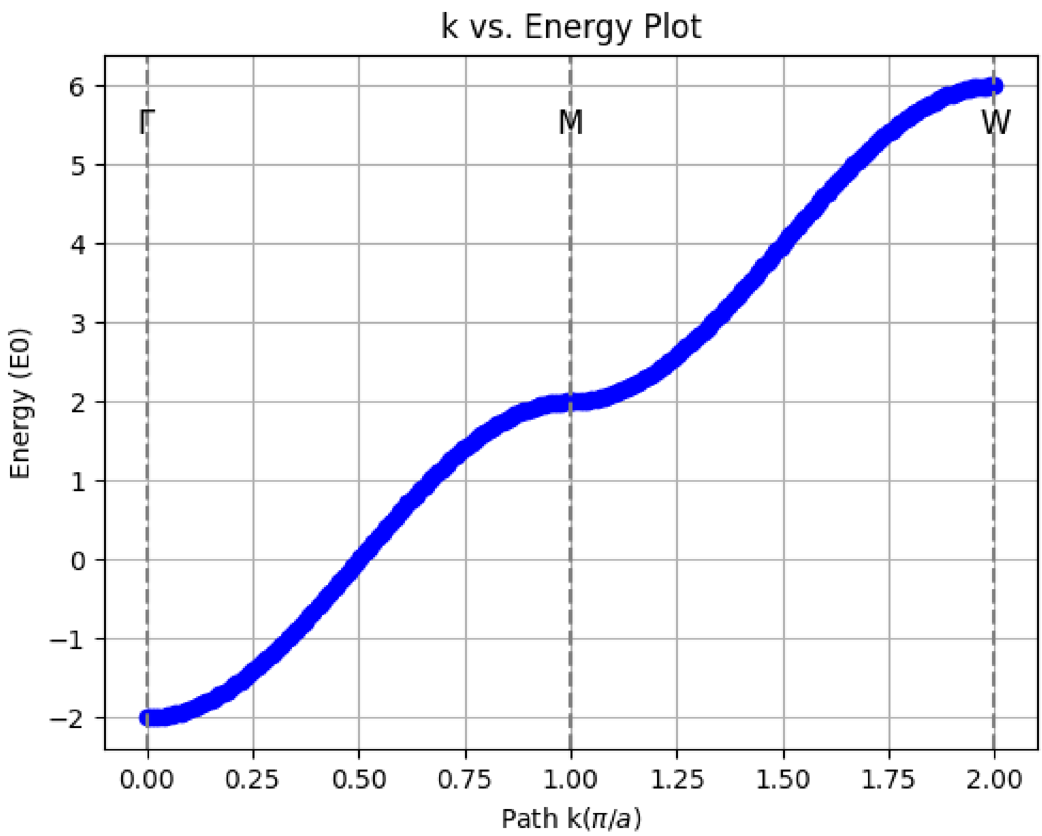
The same can be proven for

$\frac{dk_x}{dk_y} = 0$ for $k_y = \pm \frac{\pi}{a}$

$\Rightarrow$ Cross BZ with right angle.

2(d)

The k vs. energy line along the designated path is as follows



Problem 3

(a) Following A&M (10.30)

$$\det\left[\left(\varepsilon(\vec{k})\delta_{ij} - E_{s,ij}\right) + \beta_{ij} + \tilde{\gamma}_{ij}(\vec{k})\right] = 0$$

Where E_s is the original orbit energy for d and p_x, p_y, and $\beta_{ij} = 0$

$\therefore$ Only pd has non-zero matrix element,

$$\tilde{\gamma}_{ij}(\vec{k}) = \sum_{R} e^{i\vec{k}\cdot\vec{R}}\,\gamma_{ij}(\vec{R})$$

$\therefore$ The determinant looks like

$$0 = \begin{vmatrix} \varepsilon - E_p & 2t_{pd}\cos\frac{k_x a}{2} & 0 \\ 2t_{pd}\cos\frac{k_x a}{2} & \varepsilon - E_d & 2t_{pd}\cos\frac{k_y}{2}a \\ 0 & 2t_{pd}\cos\frac{k_y}{2}a & \varepsilon - E_p \end{vmatrix}$$

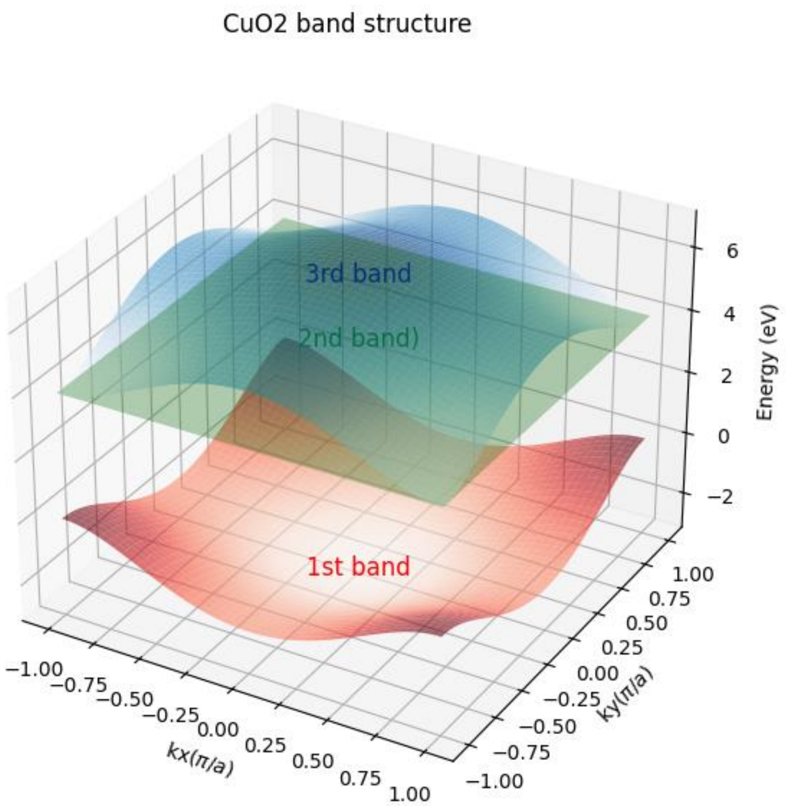
$$= (\varepsilon - E_p)\left[(\varepsilon - E_d)(\varepsilon - E_p) - 4|t_{pd}|^2\left(\cos\frac{k_y}{2}a\right)^2\right]$$

$$-4|t_{pd}|^2\left(\cos\frac{k_x a}{2}\right)^2\cdot(\varepsilon - E_p)$$

$$= (\varepsilon - E_p)^2(\varepsilon - E_d) - (\varepsilon - E_p)\left[\left(\cos\frac{k_x}{2}a\right)^2 + \left(\cos\frac{k_y}{2}a\right)^2\right]\cdot 4|t_{pd}|^2$$

3(b)

The band structure of the CuO_2 crystal is as below



3(c)

If there is only 1 electron per unit cell, it will be an insulator because there is a large bandgap between 1st and 2nd band.

If there are 2 electrons per unit cell, it will be a metal because if we look at the band structure, there are overlaps at the four edges of the Brillioun zone between the 2nd and the 3rd band.

Problem 4.

(a)

For single-atom,

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + aV_0\,\delta(x)\right]\psi(x) = 0$$

Assume $\psi(x=0) = \psi_0$

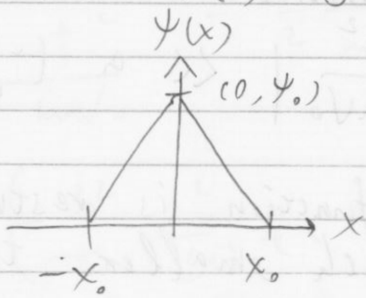
$$\therefore \quad \frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = aV_0\psi_0\,\delta(x)$$

$$\therefore \quad \frac{d^2}{dx^2}\psi(x) = 0 \quad \forall\, x \neq 0$$

$\Rightarrow$ $\psi(X)$ must be a linear function piecewise on $(-\infty, 0)$ & $(0, +\infty)$

And since $\psi(x)$ is continuous on $x=0$

$\therefore$



Assume $\psi'(x) = -\frac{\psi_0}{x_0}$ for $x_0 > x > 0$

$$\lim_{\varepsilon\to 0^+}\int_{-\varepsilon}^{+\varepsilon}\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x)\,dx = \lim_{\varepsilon\to 0^+} aV_0\psi_0\int_{-\varepsilon}^{+\varepsilon}\delta(x)\,dx$$

$$\Rightarrow \lim_{\varepsilon\to 0^+}\frac{\hbar^2}{2m}\left[\psi'(\varepsilon) - \psi'(-\varepsilon)\right] = aV_0\psi_0$$

$$\Rightarrow \quad -\frac{2\psi_0}{x_0}\cdot\frac{\hbar^2}{2m} = aV_0\psi_0 \Rightarrow x_0 = \frac{-\hbar^2}{maV_0} > 0$$

$$\therefore \psi(x) = \begin{cases} \psi_0 - \dfrac{\psi_0}{x_0}(x - x_0) & \forall x_0 \geq x \geq 0 \\ + \dfrac{\psi_0}{x_0}(x + x_0) & \forall -x_0 \leq x \leq 0 \\ 0 & \text{Otherwise} \end{cases}$$

By normalization,

$$\int |\psi|^2 dx = 1 \Rightarrow \left(\frac{\psi_0}{x_0}\right)^2 \cdot \frac{2}{3} \cdot x_0^3 = 1$$

$$\Rightarrow \psi_0 = \left(\sqrt{\frac{2}{3} x_0}\right)^{-1}$$

One thing to notice,

$$|x_0| = \left|\frac{\hbar^2}{m a V_0}\right| \ll a \quad \left(\because -V_0 \gg \frac{\hbar^2}{m a^2}\right)$$

$\therefore$ The wavefunction is restricted within an area much smaller than the lattice const.

(b)

$$\delta U = \sum_{n \neq 0} a V_0 \delta(x - na)$$

$$\therefore \beta = -\int dx \, \delta U(x) |\psi(x)|^2 = 0$$

$$\gamma(ra) = -\int dx \, \psi^*(x) \delta U(x) \psi(x - ra)$$

$$= 0 \quad (\because |x_0| \ll a)$$

no overlap of the wave functions

$$\Rightarrow \varepsilon(k) = E_s - \beta - \sum_{r \neq 0} \gamma(ra) e^{ik(ra)}$$

$= E_s$ for the lowest energy band

$\Rightarrow$ Band width $= 0$

Corresponding to the limit of strong electric potential $\Rightarrow$ Strongly localize the electrons to the individual atoms

$\Rightarrow$ Ultimate narrow bandwidth