$$\boxed{\frac{\Delta_{so}}{t'} \cong 1}$$

$$\frac{\Delta_{so}}{3}\left[\phi_{yz\uparrow} + i\,\phi_{zx\uparrow} - 1\,\phi_{xy}\downarrow\right]$$

$$\mathcal{H}_{orb} = \begin{pmatrix} \epsilon_{yz} & 0 & 0 \\ 0 & \epsilon_{zx} & 0 \\ 0 & 0 & \epsilon_{xy} \end{pmatrix} \otimes \mathbb{1}_{2\times 2}$$

$$\epsilon_{yz} \longrightarrow \qquad \Delta_{yz} + t_a'^2 \partial_x^2$$

$$\left(\mathcal{H}_{orb} + \mathcal{H}_{so}\right)\psi = E\psi$$

Example: $|yz,\uparrow\rangle$

Use notation
$$\begin{pmatrix} yz\uparrow \\ zx\uparrow \\ xy\uparrow \\ yz\downarrow \\ zx\downarrow \\ xy\downarrow \end{pmatrix} \longrightarrow \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \end{pmatrix}$$

$$g = f'$$

$$|yz\uparrow\rangle \Longrightarrow \Delta_{yz} f_1 + \underbrace{t_a'^2 f_1''}_{g_1'} + \frac{\Delta_{so}}{3}\left[f_1 + i f_2 - f_6\right] = E f_1$$

$$g_1' \quad , \quad g_1 = f_1'$$

Using $\cos(k_y a) \approx 1 - \frac{k_y^2 a^2}{2!}$, $k_y = \partial_y$

$$\mathcal{E}_{xy} = ta^2(k_x^2 + \partial_y^2)$$

$$\mathcal{E}_{yz} = t'a^2 k_x^2 + ta^2 \partial_y^2$$

$t' \approx t/_{10}$

$0 < y < L$ $\quad L \gg a$

$$\mathcal{E}_{zx} = ta^2 k_x^2 + t'a^2 \partial_y^2$$

$\mathcal{E}_{xy} = \underbrace{ta^2 k_x^2 + ta^2 \partial_y^2}_{H} + \frac{50}{3}(\ddot{-})$

$$H(k_x)\vec{\varphi}_k = \mathcal{E}_k \vec{\varphi}_k$$

$$\partial_y^2 \varphi_{xy} = \left(\frac{\mathcal{E}}{ta^2} - k_x^2\right)\varphi_{xy}$$

$$\partial_y^2 \varphi_{yz} = \left(\frac{\mathcal{E}}{ta^2} - \frac{t'}{t}k_x^2\right)\varphi_{yz}$$

$$\partial_y^2 \varphi_{zx} = \left(\frac{\mathcal{E}}{t'a^2} - \frac{t}{t'}k_x^2\right)\varphi_{zx}$$

Subject to $\vec{\varphi}(0) = 0$

Matching $\mathcal{E}$ with $\vec{\varphi}(y=L) = 0$

$a = \varphi_{xy}$ $\qquad \alpha = \mathcal{E}/_{ta^2} - k_x^2$

$b = \varphi_{yz}$ $\qquad \beta = \mathcal{E}/_{ta^2} - t'/_t\, k_x^2$

$c = \varphi_{zx}$ $\qquad \gamma = \mathcal{E}/_{t'a^2} - t/_{t'}\, k_x^2$

$$\left\{\begin{array}{l} d = a' \\ e = b' \\ f = c' \\ \\ d(0) = 1 \\ e(0) = 1 \\ f(0) = 1 \end{array}\right.$$

$\partial_y^2 a = \alpha a$

$\partial_y^2 b = \beta b$

$\partial_y^2 c = \gamma c$

$\{\, a(0) = 0 \quad b(0) = 0 \quad c(0) = 0$

$$\left\{\begin{array}{l} d' = \alpha a \\ e' = \beta b \\ f' = \gamma c \end{array}\right.$$

$\frac{\pi}{4} \to \frac{\pi}{3}$

$q \to z = y'$
$p \to y$

$z' = -\varepsilon y$
$y(0) = 0$
$z(0) = 1$
$z = y'$

4769.32

$\pi \to \frac{2\pi}{3}$

$y'' = -\varepsilon y$ $\quad y(0) = 0$, $y'(0) = 1$ $\quad y_1 = y$, $y_2 = y'$

$y_2 = y_1'$
$y_2' = -\varepsilon y_1$
$y_2(0) = 1$
$y_1(0) = 0$

$y_2'' = -y_1$

$y_1'' = y_2$

From Paul's Notes (Testing coupled DEs with EigenShooting)

$\vec{x}' = \begin{pmatrix} 1 & 2 \\ 3 & 2 \end{pmatrix} \vec{x}$ $\quad \vec{x}(0) = \begin{pmatrix} 0 \\ -4 \end{pmatrix}$

$\begin{pmatrix} y' \\ z' \end{pmatrix} = \begin{pmatrix} 1 & 2 \\ 3 & 2 \end{pmatrix} \begin{pmatrix} y \\ z \end{pmatrix}$ $\quad y(0) = 0$, $z(0) = -4$

$-a = b - c$
$+a \quad +a$
$b - c + a = 0$
$0 = -a - (-a) = b - c - (-a)$

$y' = y + 2z$
$z' = 3y + 2z$

$\vec{x}'(2) = \begin{pmatrix} -4769.32 \\ -7154.52 \end{pmatrix}$

(1) $-\frac{\partial^2}{\partial \eta^2} y + i\alpha_0 \frac{\partial}{\partial \eta} z = \tilde{\varepsilon}_n y$

$0 \le \eta \le \pi$

(2) $-\frac{\partial^2}{\partial \eta^2} z - i\alpha_0 \frac{\partial y}{\partial \eta} = \tilde{\varepsilon}_n z$

$p = y$
$q = p' \; (= y')$
$r = z$
$s = r' \; (= z')$

Trivial

(1) $\mapsto$ (3) $\quad -q' + i\alpha_0 s = \tilde{\varepsilon}_n p$

(2) $\mapsto$ (4) $\quad -s' - i\alpha_0 q = \tilde{\varepsilon}_n r$

$p(0) = 0$
$r(0) = 0$
$\left.\begin{array}{l} q(0) = 1 \\ s(0) = 1 \end{array}\right\}$ Gives non trivial solutions

Change $\tilde{\varepsilon}_n$ to Match $p(\pi) = 0$ $\; r(\pi) = 0$

Check:- $\psi'' = -E\psi$

Assume $\psi(x) = A\sin(n\pi x)$

$$\Longrightarrow -\psi(x)\left(n^2\pi^2\right) = E\psi(x)$$

$$\Longrightarrow E_n = n^2\pi^2$$

Therefore, $\boxed{\dfrac{E_n}{\pi^2} = n^2}$

Also, $A = \sqrt{2}$

$$\Longrightarrow \boxed{\psi_n(x) = \sqrt{2}\sin(n\pi x)}$$

$$-\frac{\hbar^2}{2m}\psi_\uparrow'' + \alpha i \psi_\downarrow' = \varepsilon \psi_\uparrow$$

$$f' = \frac{d}{dx} f = \frac{1}{L}\frac{d}{d\eta} f \longrightarrow f'$$

for numerical convenience

$$\psi_\sigma'' - \left(\frac{2m\alpha}{\hbar^2}\right) i\sigma \psi_{\bar\sigma}' = -\frac{2m\varepsilon}{\hbar^2}\psi_\sigma$$

$$x \in [0, 1], \qquad \sigma = \begin{cases} +1, & \uparrow \\ -1, & \downarrow \end{cases}$$

$$\bar\sigma = -\sigma$$

Define $\beta \equiv \dfrac{2m\alpha}{\hbar^2}$, and $E \equiv \dfrac{2m\varepsilon}{\hbar^2}$

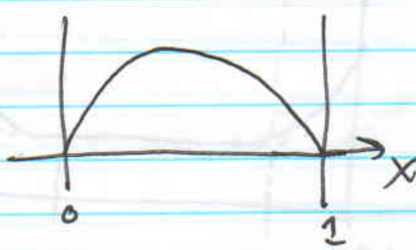
$$\Longrightarrow \boxed{\psi_\sigma'' - \beta\sigma i \psi_{\bar\sigma}' = -E\psi_\sigma}$$

$$-\partial_x^2\psi_\uparrow - i\alpha\,\partial_x\psi_\downarrow = \varepsilon\psi_\uparrow$$

$$-\partial_x^2\psi_\downarrow + i\alpha\,\partial_x\psi_\uparrow = \varepsilon\psi_\downarrow$$

$y \to$

19, 25, $\underline{\underline{32}}$



$\sin(2\pi\lambda x)$, $\lambda = 1$

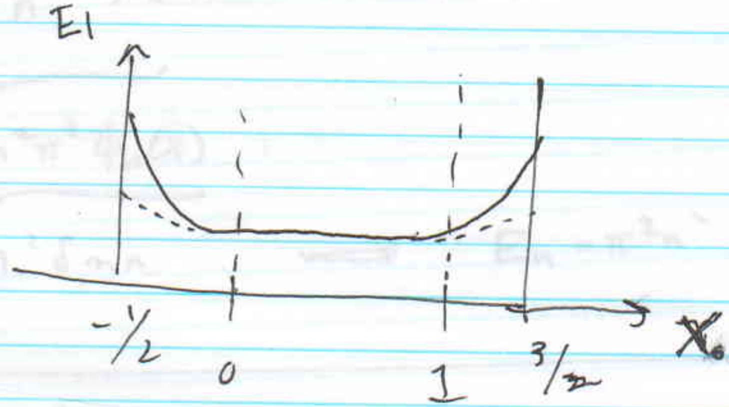
$\frac{\hbar^2}{2m} = 1$ $\qquad$ $\frac{1}{\lambda} = 2\pi$

$$\cancel{y'' - k(y-y_0)^2 = Ey^*}$$

$$y''(x) - k(x-x_0)^2\, y(x) = -E\, y(x), \quad k = \frac{1}{2}$$

$$x \in [0, 1], \quad \boxed{y(0) = 0 \ \& \ y(1) = 0}$$

$$x_0 \in [-1/2, 3/2]$$



Matrix approach (No α coupling)

$$\psi_n'' = -E_n \psi_n$$

Multiply by ψ_n^* and integrate

$$\int_0^1 \underbrace{\underbrace{\psi_m^*(x)\,\psi_n''(x)}_{-n^2\pi^2\psi_n(x)}\,dx}_{-n^2\pi^2\delta_{mn}} = -E_n\,\delta_{mn}$$

$$\Longrightarrow \quad E_n = \pi^2 n^2 \checkmark$$

Coupling term

$$\int \psi_{m\downarrow}^*(x)\left(-i\sigma\beta\right)\psi_{n\downarrow}'(x)\,dx$$

$$= -i\sigma\beta 2 \int_0^1 dx \left\{ \sin(m\pi x)\cos(n\pi x) \right\}$$

$$\cancel{= \frac{i\sigma\beta 2}{\ } \left[\frac{n - (-1)^{m+n}\, n}{m^2 - n^2} \right]}$$

$$= i\sigma\beta 2 \left[m\left(1 - (-1)^{m+n}\right) \right] \frac{n}{n^2 - m^2}$$