Note

The tight-bind Hamiltonian is rewritten as below,

$$H(k) = \begin{bmatrix} h_{11} & h_{12} \\ h_{21} & h_{22} \end{bmatrix} \tag{1}$$

where

$$h_{11} = e_g + \begin{bmatrix} 2\cos k_z V_{\text{ggd}} + 2(\cos k_x + \cos k_y)V_{\text{ggp}} & 0 & 0 \\ 0 & 2\cos k_x V_{\text{ggd}} + 2(\cos k_y + \cos k_z)V_{\text{ggp}} & 0 \\ 0 & 0 & 2\cos k_y V_{\text{ggd}} + 2(\cos k_x + \cos k_z)V_{\text{ggp}} \end{bmatrix}$$

$$h_{22} = e_f + \begin{bmatrix} 4\cos k_x V_{\text{ffp}} - 2(\cos k_y + \cos k_z)(V_{\text{ffd}} + V_{\text{ffp}}) & 0 & 0 \\ 0 & 4\cos k_y V_{\text{ffp}} - 2(\cos k_z + \cos k_x)(V_{\text{ffd}} + V_{\text{ffp}}) & 0 \\ 0 & 0 & 4\cos k_z V_{\text{ffp}} - 2(\cos k_x + \cos k_y)(V_{\text{ffd}} + V_{\text{ffp}}) \end{bmatrix}$$

$$h_{12} = 2i(V_{\text{fgd}} + V_{\text{ggp}}) \begin{bmatrix} \sin k_y & \sin k_x & 0 \\ 0 & \sin k_z & \sin k_y \\ \sin k_z & 0 & \sin k_x \end{bmatrix}; \quad h_{21} = -2i(V_{\text{fgd}} + V_{\text{ggp}}) \begin{bmatrix} \sin k_y & 0 & \sin k_z \\ \sin k_x & \sin k_z & 0 \\ 0 & \sin k_y & \sin k_x \end{bmatrix}$$

Use the approximation $2cos(\pi + \delta) = \delta^2 - 2$, $sin(\pi + \delta) = -\delta$, we can expand $H(k)$ near $k = (\pi, \pi, \pi)$ point up to the second order of k:

$$h_{11} = e_g + \begin{bmatrix} (k_z^2 - 2)V_{\text{ggd}} + (k_x^2 + k_y^2 - 4)V_{\text{ggp}} & 0 & 0 \\ 0 & (k_x^2 - 2)V_{\text{ggd}} + (k_z^2 + k_y^2 - 4)V_{\text{ggp}} & 0 \\ 0 & 0 & (k_y^2 - 2)V_{\text{ggd}} + (k_x^2 + k_z^2 - 4)V_{\text{ggp}} \end{bmatrix}$$

$$h_{22} = e_f + \begin{bmatrix} (2k_x^2 - 4)V_{\text{ffp}} - (k_y^2 + k_z^2 - 4)(V_{\text{ffd}} + V_{\text{ffp}}) & 0 & 0 \\ 0 & (2k_y^2 - 4)V_{\text{ffp}} - (k_z^2 + k_x^2 - 4)(V_{\text{ffd}} + V_{\text{ffp}}) & 0 \\ 0 & 0 & (2k_z^2 - 4)V_{\text{ffp}} - (k_x^2 + k_y^2 - 4)(V_{\text{ffd}} + V_{\text{ffp}}) \end{bmatrix}$$

$$h_{12} = -2i(V_{\text{fgd}} + V_{\text{ggp}}) \begin{bmatrix} k_y & k_x & 0 \\ 0 & k_z & k_y \\ k_z & 0 & k_x \end{bmatrix}; \quad h_{21} = 2i(V_{\text{fgd}} + V_{\text{ggp}}) \begin{bmatrix} k_y & 0 & k_z \\ k_x & k_z & 0 \\ 0 & k_y & k_x \end{bmatrix}$$

In a magnetic field, the orbital effect can be included by Peierls substitution:

$$\mathbf{k} \to \pi = \mathbf{k} + \frac{e}{\hbar}\mathbf{A} \tag{2}$$

with $\mathbf{A} = (0, B_z x, 0)$ for magnetic field along the z direction. We introduce the annihilation and creation operators and list some useful expressions below

$$a = \frac{l_c}{\sqrt{2}}\pi_-, \quad a^+ = \frac{l_c}{\sqrt{2}}\pi_+; \qquad \pi_- = \frac{\sqrt{2}}{l_c}a; \quad \pi_+ = \frac{\sqrt{2}}{l_c}a^+; \qquad \pi_x = \frac{1}{l_c\sqrt{2}}(a^+ + a); \quad \pi_y = \frac{-i}{l_c\sqrt{2}}(a^+ - a)$$

$$\pi_x^2 = \frac{1}{2l_c^2}(a^+a^+ + aa + 2a^+a + 1); \quad \pi_y^2 = -\frac{1}{2l_c^2}(a^+a^+ + aa - 2a^+a - 1); \qquad \pi_x^2 + \pi_y^2 = \frac{2}{l_c^2}(a^+a + \frac{1}{2})$$

$$[a,\ a^+] = 1; \quad a|n\rangle = \sqrt{n}|n-1\rangle; \quad a^+|n\rangle = \sqrt{n+1}|n+1\rangle; \quad a^+a|n\rangle = n|n\rangle$$

$$a^+a^+|n\rangle = a^+\sqrt{n+1}|n+1\rangle = \sqrt{(n+2)(n+1)}|n+2\rangle; \quad aa|n\rangle = a\sqrt{n}|n-1\rangle = \sqrt{n(n-1)}|n-2\rangle$$

$$\begin{array}{lllll}
\langle n|\pi_x|n-2\rangle = 0; & \langle n|\pi_x|n-1\rangle = \frac{\sqrt{n}}{l_c\sqrt{2}}; & \langle n|\pi_x|n\rangle = 0; & \langle n|\pi_x|n+1\rangle = \frac{\sqrt{n+1}}{l_c\sqrt{2}}; & \langle n|\pi_x|n+2\rangle = 0; \\
\langle n|\pi_y|n-2\rangle = 0; & \langle n|\pi_y|n-1\rangle = \frac{-i\sqrt{n}}{l_c\sqrt{2}}; & \langle n|\pi_y|n\rangle = 0; & \langle n|\pi_y|n+1\rangle = \frac{i\sqrt{n+1}}{l_c\sqrt{2}}; & \langle n|\pi_y|n+2\rangle = 0; \\
\langle n|\pi_x^2|n-2\rangle = \frac{\sqrt{n(n-1)}}{2l_c^2}; & \langle n|\pi_x^2|n-1\rangle = 0; & \langle n|\pi_x^2|n\rangle = \frac{2n+1}{2l_c^2}; & \langle n|\pi_x^2|n+1\rangle = 0; & \langle n|\pi_x^2|n+2\rangle = \frac{\sqrt{(n+1)(n+2)}}{2l_c^2}; \\
\langle n|\pi_y^2|n-2\rangle = \frac{-\sqrt{n(n-1)}}{2l_c^2}; & \langle n|\pi_y^2|n-1\rangle = 0; & \langle n|\pi_y^2|n\rangle = \frac{2n+1}{2l_c^2}; & \langle n|\pi_y^2|n+1\rangle = 0; & \langle n|\pi_y^2|n+2\rangle = \frac{-\sqrt{(n+1)(n+2)}}{2l_c^2}; \\
\langle n|c|n-2\rangle = 0 & \langle n|c|n-1\rangle = 0 & \langle n|c|n\rangle = c & \langle n|c|n+1\rangle = 0 & \langle n|c|n+2\rangle = 0
\end{array}$$

where $l_c = \sqrt{\hbar/eB_z} = 1/\sqrt{B}$. (Let $\hbar = e = 1$) and $|n\rangle$ is the harmonic oscillator function.
At $k_z = 0$, Hamiltonian (1) can are written as:

$$\langle n|H|n\rangle = DiagForm\begin{bmatrix} E_g - 2V_{\text{ggd}} + \big(B(2n+1) - 4\big)V_{\text{ggp}} \\ E_g + (\frac{2n+1}{2}B - 2)V_{\text{ggd}} + (\frac{2n+1}{2}B - 4)V_{\text{ggp}} \\ E_g + (\frac{2n+1}{2}B - 2)V_{\text{ggd}} + (\frac{2n+1}{2}B - 4)V_{\text{ggp}} \\ E_f + ((2n+1)B - 4)V_{\text{ffp}} - (\frac{2n+1}{2}B - 4)(V_{\text{ffd}} + V_{\text{ffp}}) \\ E_f + ((2n+1)B - 4)V_{\text{ffp}} - (\frac{2n+1}{2}B - 4)(V_{\text{ffd}} + V_{\text{ffp}}) \\ E_f - 4V_{\text{ffp}} - (B(2n+1) - 4)(V_{\text{ffd}} + V_{\text{ffp}}) \end{bmatrix}$$

$$\langle n|H|n+1\rangle = 2i(V_{\text{fgd}} + V_{\text{ggp}})\begin{bmatrix} 0 & 0 & 0 & -i\sqrt{B(n+1)/2} & -\sqrt{B(n+1)/2} & 0 \\ 0 & 0 & 0 & 0 & 0 & -i\sqrt{B(n+1)/2} \\ 0 & 0 & 0 & 0 & 0 & -\sqrt{B(n+1)/2} \\ i\sqrt{B(n+1)/2} & 0 & 0 & 0 & 0 & 0 \\ \sqrt{B(n+1)/2} & 0 & 0 & 0 & 0 & 0 \\ 0 & i\sqrt{B(n+1)/2} & \sqrt{B(n+1)/2} & 0 & 0 & 0 \end{bmatrix}$$

$$\langle n|H|n+2\rangle = DiagForm\begin{bmatrix} 0 \\ \frac{B\sqrt{(n+1)(n+2)}}{2}V_{\text{ggd}} - \frac{B\sqrt{(n+1)(n+2)}}{2}V_{\text{ggp}} \\ \frac{-B\sqrt{(n+1)(n+2)}}{2}V_{\text{ggd}} + \frac{B\sqrt{(n+1)(n+2)}}{2}V_{\text{ggp}} \\ B\sqrt{(n+1)(n+2)}V_{\text{ffp}} + \frac{B\sqrt{(n+1)(n+2)}}{2}(V_{\text{ffd}} + V_{\text{ffp}}) \\ -B\sqrt{(n+1)(n+2)}V_{\text{ffp}} - (\frac{B\sqrt{(n+1)(n+2)}}{2})(V_{\text{ffd}} + V_{\text{ffp}}) \\ 0 \end{bmatrix}$$

the total Hamiltonian is

$$H = \begin{bmatrix} \langle 0|H|0\rangle & \langle 0|H|1\rangle & \langle 0|H|2\rangle & 0 & 0 & 0 & ... \\ & \langle 1|H|1\rangle & \langle 1|H|2\rangle & \langle 1|H|3\rangle & 0 & 0 & ... \\ & & \langle 2|H|2\rangle & \langle 2|H|3\rangle & \langle 2|H|4\rangle & 0 & ... \\ & & & \langle 3|H|3\rangle & \langle 3|H|4\rangle & \langle 3|H|5\rangle & ... \\ & & & & ... & ... & ... \\ & \dagger & & & & ... & ... \\ & & & & & & ... \end{bmatrix} \tag{3}$$

The Landau level can be calculated form eq(3). The calculation results are shown in Fig.1 and 2.

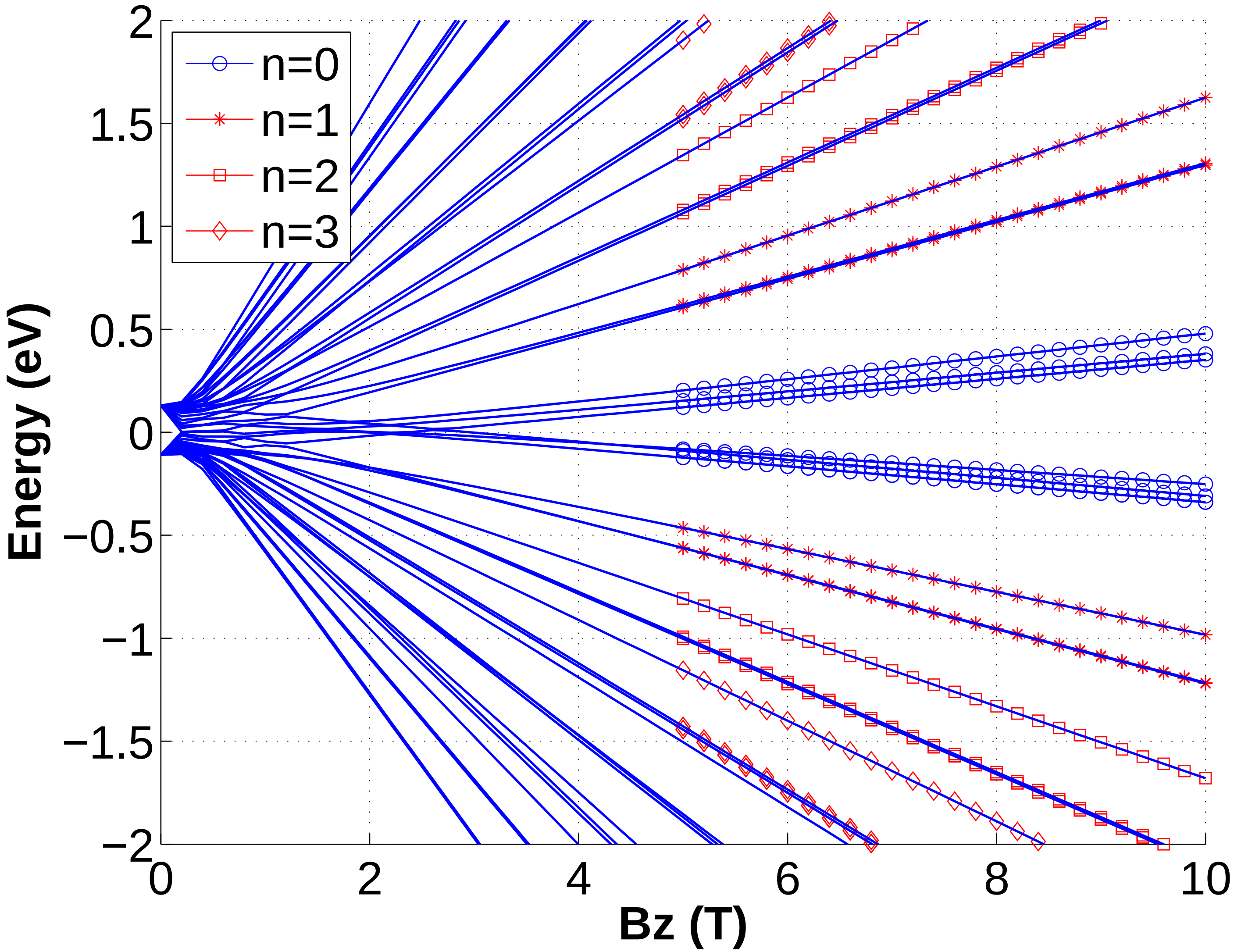

Figure 1: Landau energy vs. B

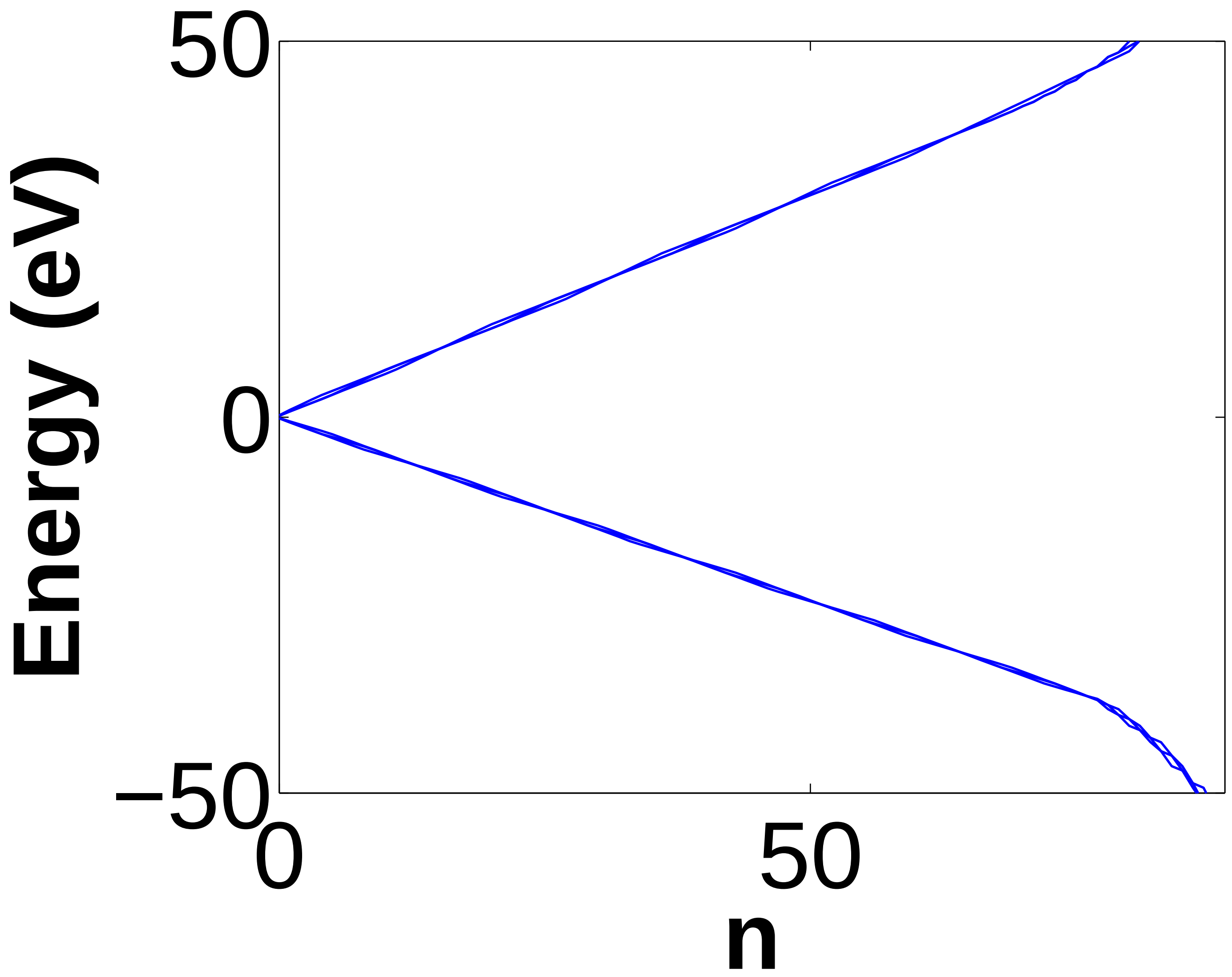

Figure 2: Landau energy vs. n