Landau Level in node line system

April 15, 2014

case one: node line on the kx-ky plane:

The simplest 2x2 Hamiltonian to describe the node line structure can be written as:

$$H = \big[-\epsilon_0 + \alpha(k_x^2 + k_y^2 + k_z^2)\big]\sigma_z + \beta k_z \sigma_x = \begin{bmatrix} -\epsilon_0 + \alpha(k_x^2 + k_y^2 + k_z^2) & \beta k_z \\ \beta k_z & \epsilon_0 - \alpha(k_x^2 + k_y^2 + k_z^2) \end{bmatrix} \tag{1}$$

where $\epsilon_0 > 0$, $\alpha > 0$. The diagonal term$\pm\big[-\epsilon_0 + \alpha(k_x^2 + k_y^2 + k_z^2)\big]$ are two parabolic like free electrons which construct a band inversion structure. At $k_z = 0$ plane, there is a node line at $(k_x^2 + k_y^2) = \epsilon_0/\alpha$. Fit to the tight binding dispersion we have $\epsilon_0 = 0.12$ eV, $\alpha = 7.24411\ eV \cdot A^2$, $\beta = 0.690696\ eV \cdot A$ (considered the lattice parameter $a = 14.48$ angstrom). The comparison between tight binding results and the 2x2 model are shown in Fig.1. The band dispersion are plotted near the one node line point on the x axis.

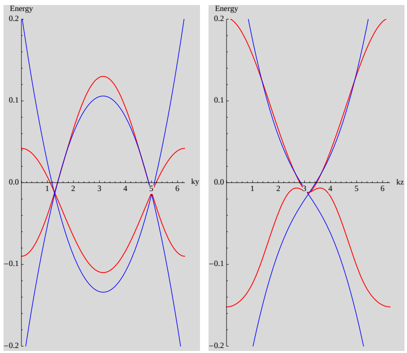

Figure 1: compare the results form tight-binding (red line) and 2x2 model (blue line) near the node line. left: along ky direction, right: along kz direction.

In a magnetic field, the orbital effect can be included by Peierls substitution $\mathbf{k} \to \pi = \mathbf{k} + \frac{e}{\hbar}\mathbf{A}$, 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

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

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

$$\begin{array}{lll} \langle n|\pi_x|n-1\rangle = \frac{\sqrt{n}}{l_c\sqrt{2}}; & \langle n|\pi_x|n\rangle = 0; & \langle n|\pi_x|n+1\rangle = \frac{\sqrt{n+1}}{l_c\sqrt{2}}; \\ \langle n|\pi_y|n-1\rangle = \frac{-i\sqrt{n}}{l_c\sqrt{2}}; & \langle n|\pi_y|n\rangle = 0; & \langle n|\pi_y|n+1\rangle = \frac{i\sqrt{n+1}}{l_c\sqrt{2}}; \end{array} \tag{2}$$

where $l_c = \sqrt{\hbar/eB_z}$ and $|n\rangle$ is the harmonic oscillator function. The Hamiltonian can be written as,

$$H = \begin{bmatrix} -\epsilon_0 + \alpha(\pi_x^2 + \pi_y^2) + \alpha k_z^2 & \beta k_z \\ \beta k_z & \epsilon_0 - \alpha(\pi_x^2 + \pi_y^2) - \alpha k_z^2 \end{bmatrix} \tag{3}$$

$$H = \begin{bmatrix} -\epsilon_0 + 2\alpha B_z(n + \frac{1}{2})\frac{e}{\hbar} + \alpha k_z^2 & \beta k_z \\ \beta k_z & \epsilon_0 - 2\alpha B_z(n + \frac{1}{2})\frac{e}{\hbar} - \alpha k_z^2 \end{bmatrix} \tag{4}$$

$$E_{n,\pm} = \pm\sqrt{(\epsilon_0 - \alpha B_z(2n+1)\frac{e}{\hbar} - \alpha k_z^2)^2 + \beta^2 k_z^2} \tag{5}$$

The energy of Landau level as a function of B_z is shown in Fig. 2.

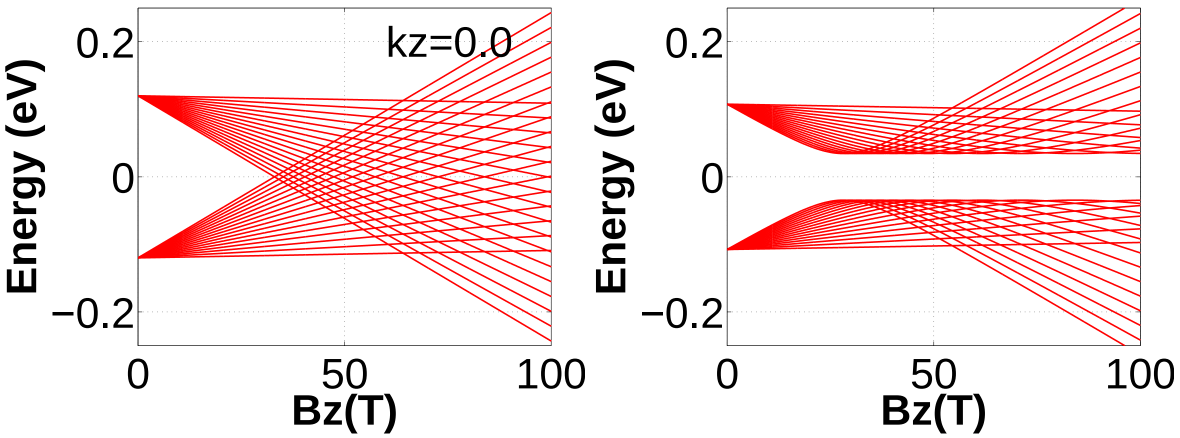

Figure 2: LL in the case of node line on the $k_x k_y$ plane. left, $k_z = 0$, right, $k_z = 0.05\ A^{-1}$.

case two: node line on the ky-kz plane:

The simplest 2x2 Hamiltonian to describe the node line structure can be written as:

$$H = \begin{bmatrix} -\epsilon_0 + \alpha(k_x^2 + k_y^2 + k_z^2) & \beta k_x \\ \beta k_x & \epsilon_0 - \alpha(k_x^2 + k_y^2 + k_z^2) \end{bmatrix} \tag{6}$$

In a magnetic field along the z direction, with $\mathbf{A} = (0, B_z x, 0)$, we have

$$H = \begin{bmatrix} -\epsilon_0 + \alpha(\pi_x^2 + \pi_y^2 + k_z^2) & \beta \pi_x \\ \beta \pi_x & \epsilon_0 - \alpha(\pi_x^2 + \pi_y^2 + k_z^2) \end{bmatrix} \tag{7}$$

$$H = \begin{bmatrix} -\epsilon_0 + 2\alpha B_z(a^+ a + \frac{1}{2})\frac{e}{\hbar} + \alpha k_z^2 & \beta\sqrt{\frac{eB_z}{2\hbar}}(a^+ + a) \\ \beta\sqrt{\frac{eB_z}{2\hbar}}(a^+ + a) & \epsilon_0 - 2\alpha B_z(a^+ a + \frac{1}{2})\frac{e}{\hbar} - \alpha k_z^2 \end{bmatrix} \tag{8}$$

We can get

$$\langle n|H|n\rangle = \begin{bmatrix} -\epsilon_0 + \alpha B_z(2n+1)\frac{e}{\hbar} + \alpha k_z^2 & 0 \\ 0 & \epsilon_0 - \alpha B_z(2n+1)\frac{e}{\hbar} - \alpha k_z^2 \end{bmatrix} \tag{9}$$

$$\langle n|H|n+1\rangle = \begin{bmatrix} 0 & \beta\sqrt{(n+1)\frac{eB_z}{2\hbar}} \\ \beta\sqrt{(n+1)\frac{eB_z}{2\hbar}} & 0 \end{bmatrix} \tag{10}$$

with above two equations, we can write the Hamiltonian matrix as below,

$$H = \begin{bmatrix} \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \cdots \\ \cdots & E_{n-1,-} & 0 & 0 & \beta\sqrt{\frac{neB_z}{2\hbar}} & 0 & 0 & 0 & 0 & \cdots \\ \cdots & 0 & E_{n-1,+} & \beta\sqrt{\frac{neB_z}{2\hbar}} & 0 & 0 & 0 & 0 & 0 & \cdots \\ \cdots & 0 & \beta\sqrt{\frac{neB_z}{2\hbar}} & E_{n,-} & 0 & 0 & \beta\sqrt{\frac{(n+1)eB_z}{2\hbar}} & 0 & 0 & \cdots \\ \cdots & \beta\sqrt{\frac{neB_z}{2\hbar}} & 0 & 0 & E_{n,+} & \beta\sqrt{\frac{(n+1)eB_z}{2\hbar}} & 0 & 0 & 0 & \cdots \\ \cdots & 0 & 0 & 0 & \beta\sqrt{\frac{(n+1)eB_z}{2\hbar}} & E_{n+1,-} & 0 & 0 & \beta\sqrt{\frac{(n+2)eB_z}{2\hbar}} & \cdots \\ \cdots & 0 & 0 & \beta\sqrt{\frac{(n+1)eB_z}{2\hbar}} & 0 & 0 & E_{n+1,+} & \beta\sqrt{\frac{(n+2)eB_z}{2\hbar}} & 0 & \cdots \\ & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \cdots \end{bmatrix} \tag{11}$$

where $E_{n,\pm} = \pm\left(\epsilon_0 - \alpha(2n+1)B_z\frac{e}{\hbar} - \alpha k_z^2\right)$.

- If $\beta = 0$, the Hamiltonian is diagonal and the eigenvalues are

$$E_{n,\pm} = \pm\left(\epsilon_0 - \alpha(2n+1)B_z\frac{e}{\hbar} - \alpha k_z^2\right) \tag{12}$$

and the eigen-vectors are ϕ_n for $E_{n,+}$ and ψ_n for $E_{n,-}$. The LL $E_{n,+}$and $E_{n,-}$ cross at $B_z = \frac{\epsilon_0 - \alpha k_z^2}{\alpha(2n+1)}\frac{\hbar}{e}$ if $\epsilon_0 - \alpha k_z^2 > 0$ as shown in fig 4 ($\beta = 0$).

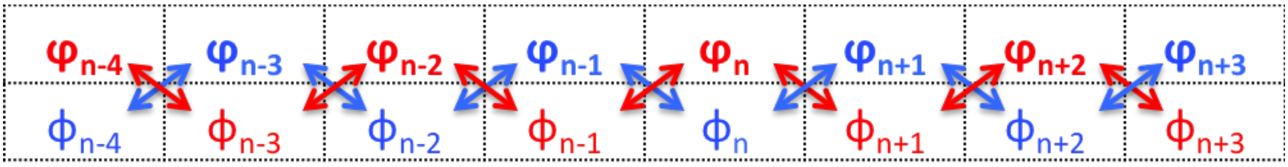

Figure 3: the β terms coupled the states with blue or red states, but there is no coupling between red and blue color states.

- If $\beta \neq 0$, we can see from eq(11) that these β terms couples ψ_n (ϕ_n) and $\phi_{n\pm1}$ ($\psi_{n\pm1}$) as shown in fig.3. We can see that there is no coupling between ϕ_n and ψ_n sub-bands, then the crossing point between $E_{n,+}$ and $E_{n,-}$ are remain as shown in Fig.4. We take the the figure with $\beta = 0.1\beta_{real}$ as an example, the landau level cross points are between (ψ_1, ϕ_1),(ψ_2, ϕ_2),(ψ_3, ϕ_3),(ψ_4, ϕ_4)..., because there are no coupling between them.

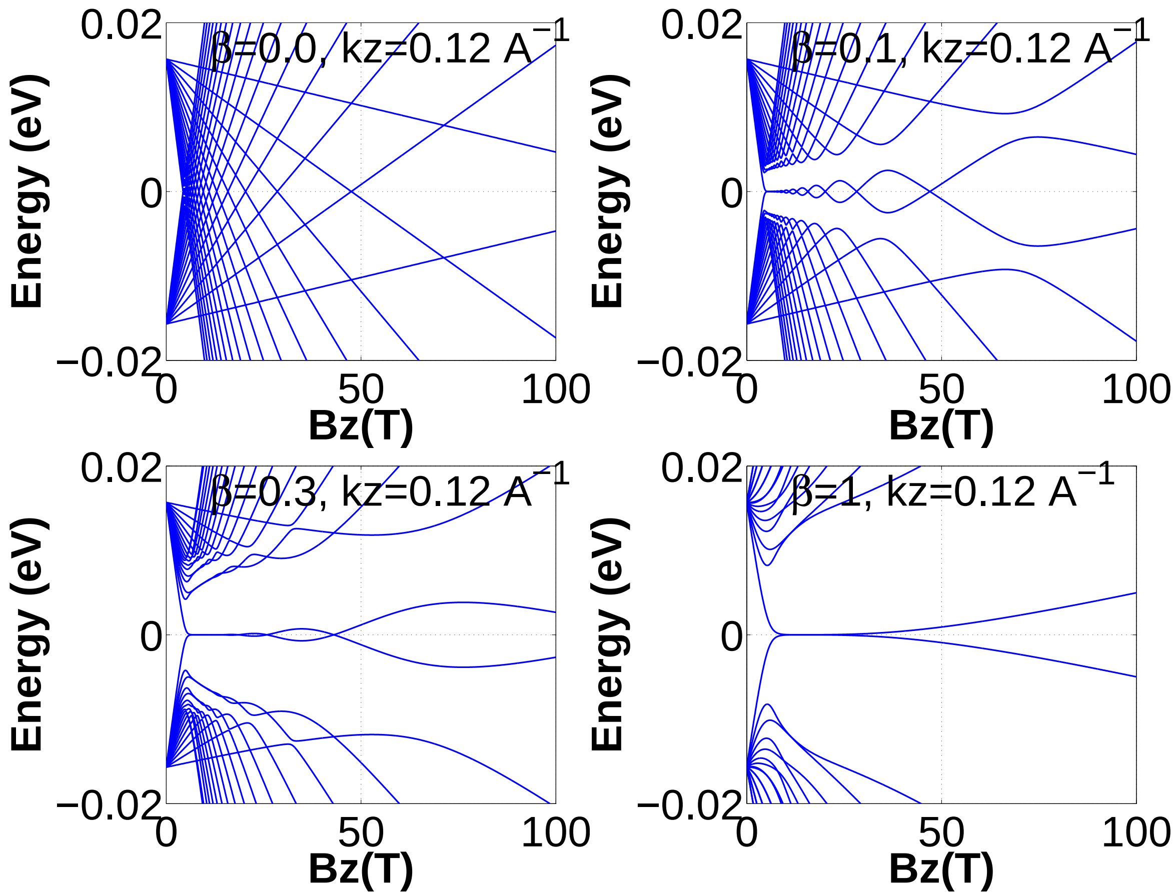

Figure 4: LL in the case of node line on the k$_y$k$_z$ plane. Here we set $k_z = 0.12$ 1/angstrom, and tune β values with 0, $0.1\beta_{real}$, $0.3\beta_{real}$, and β_{real}.