# Tight Binding Based modelling of bilayer graphene

1. Tight binding theory

When electron is tightly bounded to nucleus, it is useful to express wavefunction in terms of one atom wavefunction basis.

The wavefunction with band index j satisfying the Bloch condition can be expressed as

$$\left| \Psi_{j\mathbf{k}} \right\rangle = \frac{1}{\sqrt{N}} \sum_{p} \sum_{\mathbf{R}_i} e^{i\mathbf{k}\cdot(\mathbf{R}_i + \boldsymbol{\delta}_p)} c_j^p(\mathbf{k}) \left| \phi^p, \mathbf{R}_i + \boldsymbol{\delta}_p \right\rangle \tag{1}$$

where N is total number of unit cells and p is the index for atom type in the unit cell and $\mathbf{R}_i$ is a lattice vector. $\boldsymbol{\delta}_p$ describes the position of atom p in the unit cell and $\left| \varphi^p, \mathbf{R} + \boldsymbol{\delta}_p \right\rangle$ is the one atom π orbital wavefunction of atom p centered on $\mathbf{R}_i + \boldsymbol{\delta}_p$. In case of bilayer graphene, we are only interested in π orbital electron. Thus I omitted the summation over energy level of one atom. The lattice structure of bilayer graphene is described below.
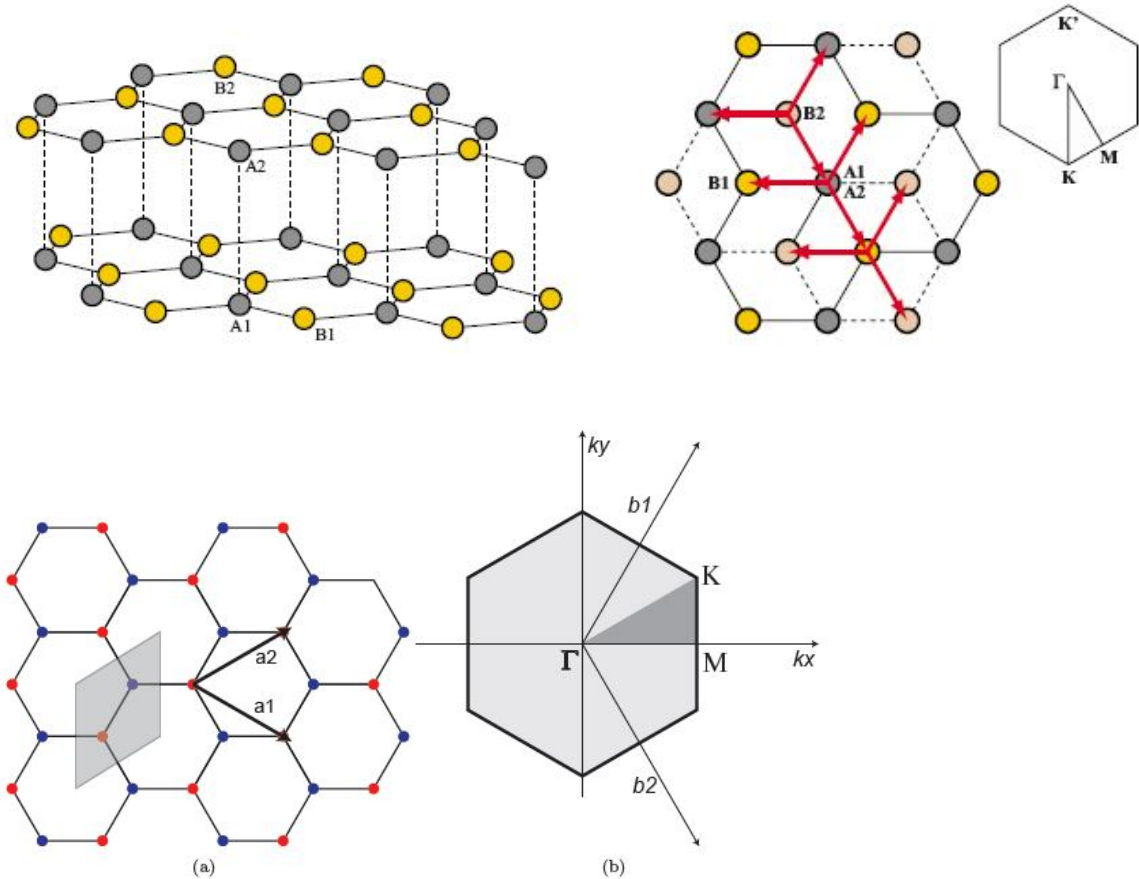
From the figure, you can see that p can be A1, B1, A2, B2. Then p'th bloch function is given by

$$\left|\Phi_{\mathbf{k}}^{p}\right\rangle = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}_i} e^{i\mathbf{k}\cdot(\mathbf{R}_i+\boldsymbol{\delta}_p)} \left|\varphi^{p}, \mathbf{R}_p + \boldsymbol{\delta}_p\right\rangle \tag{2}$$

Using p'th bloch function, total wavefunction can be written as

$$\left|\Psi_{j\mathbf{k}}\right\rangle = \sum_{p} c_j^{p}(\mathbf{k}) \left|\Phi_{\mathbf{k}}^{p}\right\rangle \tag{3}$$

In order to determine $c_j^{p}(\mathbf{k})$, the wavefunction is inserted into Schrödinger equation

$$\hat{H}\left|\Psi_{j\mathbf{k}}\right\rangle = E_j(\mathbf{k})\left|\Psi_{j\mathbf{k}}\right\rangle \tag{4}$$

By using eqn (3), one gets

$$\sum_{p} c_j^{p}(\mathbf{k})\hat{H}\left|\Phi_{\mathbf{k}}^{p}\right\rangle = E_j(\mathbf{k})\sum_{p} c_j^{p}(\mathbf{k})\left|\Phi_{\mathbf{k}}^{p}\right\rangle \tag{5}$$

Acting $\left\langle\Phi_{\mathbf{k}}^{p'}\right|$ gives

$$\sum_{p} c_j^{p}(\mathbf{k})\left\langle\Phi_{\mathbf{k}}^{p'}\left|\hat{H}\right|\Phi_{\mathbf{k}}^{p}\right\rangle = E_j(\mathbf{k})\sum_{p} c_j^{p}(\mathbf{k})\left\langle\Phi_{\mathbf{k}}^{p'}\left|\Phi_{\mathbf{k}}^{p}\right.\right\rangle \tag{6}$$

This can be written as matrix form

$$\hat{\mathrm{H}}\cdot\vec{c}_j = E_j(\mathbf{k})\cdot\hat{\mathrm{S}}\cdot\vec{c}_j \tag{7}$$

Matrix element of $\hat{\mathrm{H}}$ and $\hat{\mathrm{S}}$ is given by

$$\hat{\mathrm{H}}_{p'p} = \left\langle\Phi_{\mathbf{k}}^{p'}\left|\hat{H}\right|\Phi_{\mathbf{k}}^{p}\right\rangle$$

$$= \frac{1}{N}e^{i\mathbf{k}\cdot(\boldsymbol{\delta}_p-\boldsymbol{\delta}_{p'})}\sum_{\mathbf{R}_j}\sum_{\mathbf{R}_i} e^{i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\left\langle\varphi^{p'}, \mathbf{R}_j + \boldsymbol{\delta}_{p'}\left|\hat{H}\right|\varphi^{p}, \mathbf{R}_i + \boldsymbol{\delta}_p\right\rangle$$

$$= \sum_{\mathbf{R}_i} e^{i\mathbf{k}\cdot(\mathbf{R}_i+\boldsymbol{\delta}_p-\boldsymbol{\delta}_{p'})}\left\langle\varphi^{p'}, \vec{0} + \boldsymbol{\delta}_{p'}\left|\hat{H}\right|\varphi^{p}, \mathbf{R}_i + \boldsymbol{\delta}_p\right\rangle \tag{8}$$

$$\hat{S}_{p'p} = \left\langle \Phi_{\mathbf{k}}^{p'} \middle| \Phi_{\mathbf{k}}^{p} \right\rangle$$

$$= \frac{1}{N} e^{i\mathbf{k}\cdot(\boldsymbol{\delta}_p - \boldsymbol{\delta}_{p'})} \sum_{\mathbf{R}_j} \sum_{\mathbf{R}_i} e^{i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)} \left\langle \varphi^{p'}, \mathbf{R}_j + \boldsymbol{\delta}_{p'} \middle| \varphi^{p}, \mathbf{R}_i + \boldsymbol{\delta}_p \right\rangle$$

$$= e^{i\mathbf{k}\cdot(\boldsymbol{\delta}_p - \boldsymbol{\delta}_{p'})} \sum_{\mathbf{R}_i} e^{i\mathbf{k}\cdot\mathbf{R}_i} \left\langle \varphi^{p'}, \vec{0} + \boldsymbol{\delta}_{p'} \middle| \varphi^{p}, \mathbf{R}_i + \boldsymbol{\delta}_p \right\rangle$$

(9)

2. Approximations in tight binding

So far, everything is exact. Here comes the approximation. First, We assume that $\hat{S} = I$, i.e., the overlap between one atom wavefunctions centered on different position is ignored. Then equation (7) becomes usual eigenvalue problem.

$$\hat{H} \cdot \vec{c}_j = E_j(\mathbf{k}) \cdot \vec{c}_j$$

(10)

Second, when we calculate the component of $\hat{H}$, we only consider interaction between the nearest neighbors, i.e., $\left\langle \varphi^{p'}, \vec{0} + \boldsymbol{\delta}_{p'} \middle| \hat{H} \middle| \varphi^{p}, \mathbf{R}_i + \boldsymbol{\delta}_p \right\rangle$ is 0 unless $\boldsymbol{\delta}_{p'}$ and $\mathbf{R}_i + \boldsymbol{\delta}_p$ are the nearest neighbors.

3. Bilayer graphene band structure

Now we are ready to calculate band structure of bilayer graphene. From the figure below, the lattice vectors of the bilayer graphene lattice are given by

$$a_1 = (\frac{\sqrt{3}}{2}, \frac{1}{2}, 0)a_0, \qquad a_2 = (\frac{\sqrt{3}}{2}, -\frac{1}{2}, 0)a_0 \quad \text{where} \quad a_0 \text{ is lattice constant}$$

(11)

(a)   (b)
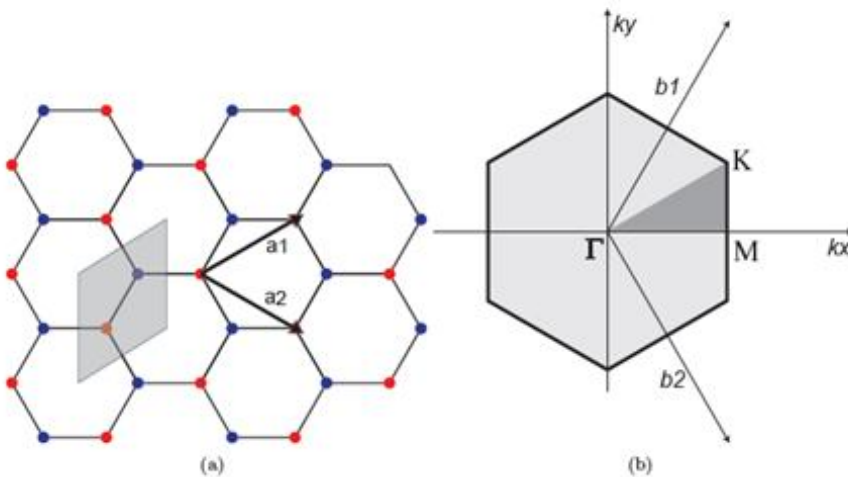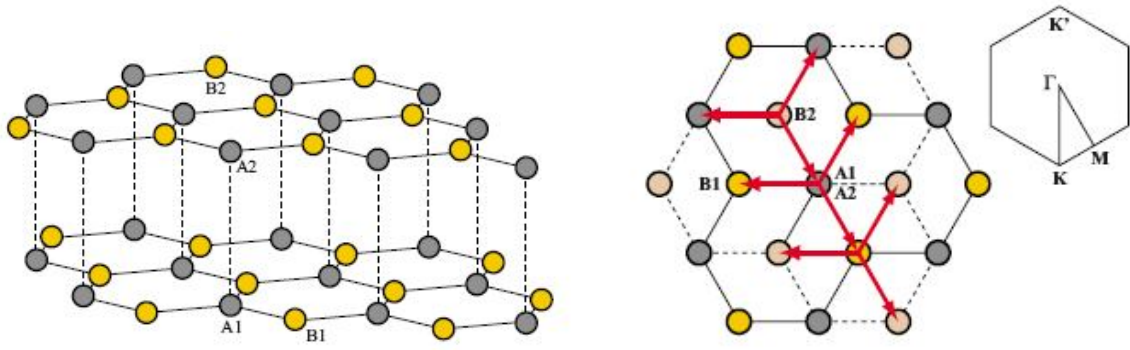
Since there are four atoms in the basis, there are four Bloch functions. Let's denote four atoms by A1,B1,A2,B2. A1,B2 are in lower plane and A2, B2 are in upper plane. Thus $\hat{H}$ is 4 by 4 matrix and the matrix element is given by

$$\hat{H}_{A1,A1} = \hat{H}_{B1,B1} = \left\langle \Phi_{\mathbf{k}}^{A1} \middle| \hat{H} \middle| \Phi_{\mathbf{k}}^{A1} \right\rangle = \left\langle \varphi, \vec{0} + \boldsymbol{\delta}_{A1} \middle| \hat{H} \middle| \varphi, \vec{0} + \boldsymbol{\delta}_{A1} \right\rangle = \varepsilon_1$$

$$\hat{H}_{A2,A2} = \hat{H}_{B2,B2} = \left\langle \Phi_{\mathbf{k}}^{A2} \middle| \hat{H} \middle| \Phi_{\mathbf{k}}^{A2} \right\rangle = \left\langle \varphi, \vec{0} + \boldsymbol{\delta}_{A2} \middle| \hat{H} \middle| \varphi, \vec{0} + \boldsymbol{\delta}_{A2} \right\rangle = \varepsilon_2$$

$$\hat{H}_{A1,B1} = \hat{H}_{A2,B2} = \left\langle \Phi_{\mathbf{k}}^{A1} \middle| \hat{H} \middle| \Phi_{\mathbf{k}}^{B1} \right\rangle = \left\langle \Phi_{\mathbf{k}}^{B1} \middle| \hat{H} \middle| \Phi_{\mathbf{k}}^{A1} \right\rangle^{*}$$

$$= -\gamma_0 (e^{i\mathbf{k}\cdot\mathbf{r}_1} + e^{i\mathbf{k}\cdot\mathbf{r}_2} + e^{i\mathbf{k}\cdot\mathbf{r}_3}) = -\gamma_0 f_1(\mathbf{k})$$

$$\hat{H}_{A1,A2} = \left\langle \Phi_{\mathbf{k}}^{A1} \middle| \hat{H} \middle| \Phi_{\mathbf{k}}^{A2} \right\rangle = -\gamma_1 e^{i\mathbf{k}\cdot\mathbf{r}_4}$$

$$\text{where } -\gamma_0 = \left\langle \varphi^{A1}, \boldsymbol{\delta}_{A1} \middle| \hat{H} \middle| \varphi^{A1}, \boldsymbol{\delta}_{A1} + \mathbf{r}_1 \right\rangle, \quad -\gamma_1 = \left\langle \varphi^{A1}, \boldsymbol{\delta}_{A1} \middle| \hat{H} \middle| \varphi^{A2}, \boldsymbol{\delta}_{A1} + \mathbf{r}_4 \right\rangle$$

(12)

Here $\mathbf{r}_i$ is the vectors connecting the nearest neighbors which are given by

$$\mathbf{r}_1 = (\frac{1}{2\sqrt{3}}, \frac{1}{2}, 0)a_0, \quad \mathbf{r}_2 = (\frac{1}{2\sqrt{3}}, -\frac{1}{2}, 0)a_0, \quad \mathbf{r}_3 = (-\frac{1}{\sqrt{3}}, 0, 0)a_0, \quad \mathbf{r}_4 = (0, 0, 1)b_0 \tag{13}$$

Here b_0 is the distance between planes. Using (13), $f_1(\mathbf{k})$ and $e^{i\mathbf{k}\cdot\mathbf{r}_4}$ can be written as

$$f_1(\mathbf{k}) = e^{-ik_x a_0 / \sqrt{3}} + 2e^{ik_x a_0 /(2\sqrt{3})} \cos(k_y a_0 / 2)$$

$$e^{i\mathbf{k}\cdot\mathbf{r}_4} = 1$$

(14)

To sum up, energy band are given by eigenvalues of $\hat{H}$ given by

$$
\hat{H} = \begin{array}{c} \\ \langle A1| \\ \langle B1| \\ \langle A2| \\ \langle B2| \end{array}
\begin{array}{cccc}
|A1\rangle & |B1\rangle & |A2\rangle & |B2\rangle
\end{array}
\left(
\begin{array}{cccc}
-\Delta/2 & -\gamma_0 f_1(\mathbf{k}) & -\gamma_1 & 0 \\
-\gamma_0 f_1(\mathbf{k})* & -\Delta/2 & 0 & 0 \\
-\gamma_1 & 0 & \Delta/2 & -\gamma_0 f_1(\mathbf{k}) \\
0 & 0 & -\gamma_0 f_1(\mathbf{k})* & \Delta/2
\end{array}
\right)
\tag{15}
$$

$$
\text{where } \Delta = \varepsilon_2 - \varepsilon_1
$$

In (15) I set $\varepsilon_1 = -\Delta/2 \Leftrightarrow \varepsilon_1 = -\varepsilon_2$ (In only causes a shift of eigenvalues). In order to calculate band structure the reciprocal vectors have to be known. The reciprocal vectors $\mathbf{b}_i$ are calculated by requiring $\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi \delta_{ij}$. The reciprocal vectors are found to be
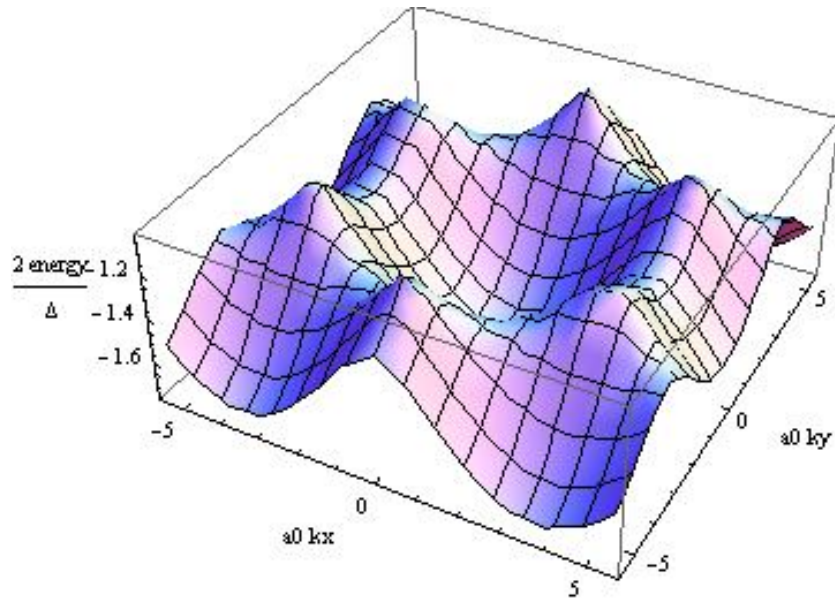
$$
\mathbf{b}_1 = (\frac{1}{\sqrt{3}}, 1)\frac{2\pi}{a_0}, \quad \mathbf{b}_2 = (\frac{1}{\sqrt{3}}, -1)\frac{2\pi}{a_0}
\tag{16}
$$

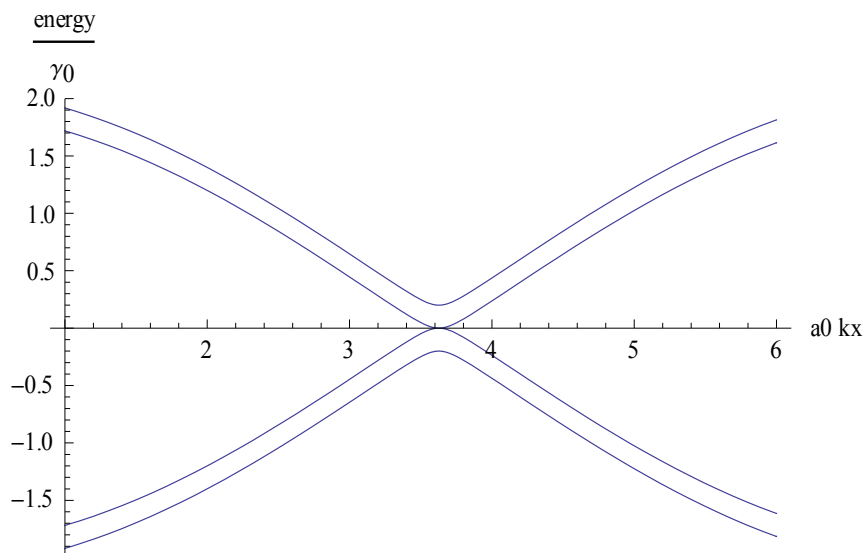From the reciprocal vectors the first Brillouin zone can be found. Below figure is describing Brillouin zone.
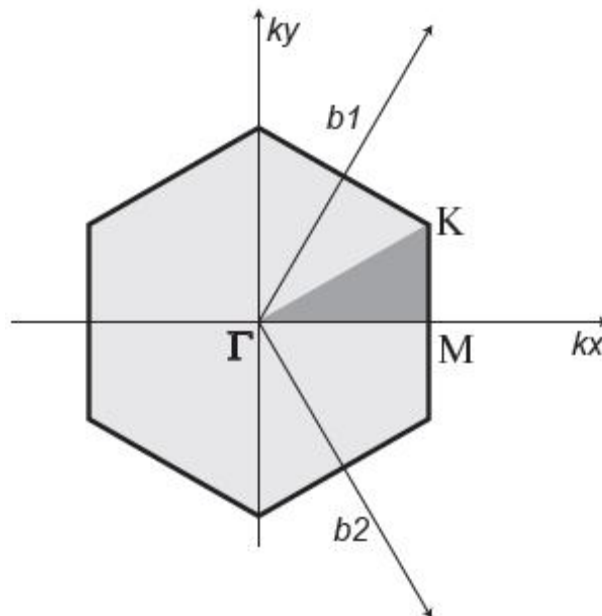
$K = (\dfrac{2\pi}{\sqrt{3}a_0}, \dfrac{2\pi}{3a_0})$ in the figure is called Dirac point.
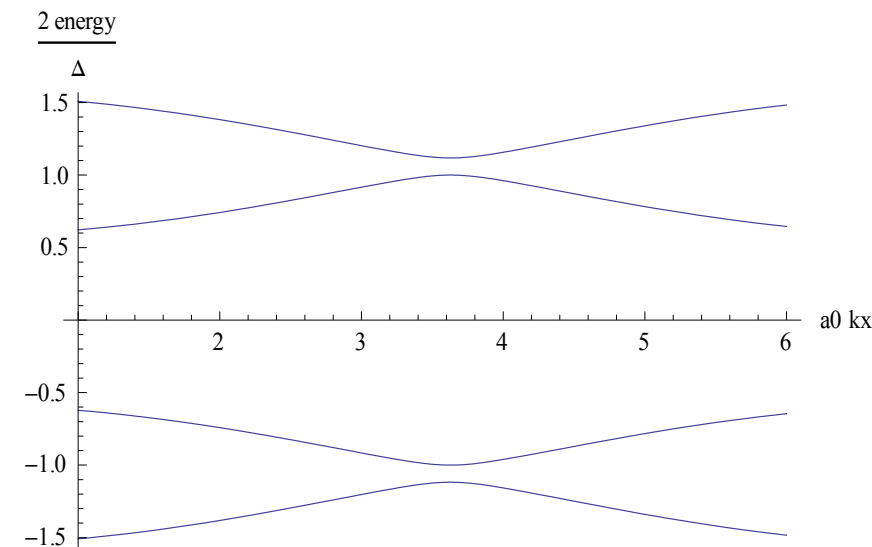
Graph of band structure is like below.

$$\frac{\gamma_0}{\Delta/2} = 0.25, \quad \frac{\gamma_1}{\gamma_0} = 0.2$$

$$\Delta = 0, \quad \frac{\gamma_1}{\gamma_0} = 0.2, \quad k_y = \frac{2\pi}{3a_0}$$

(graph near Dirac Point)

$$\frac{\gamma_0}{\Delta/2} = 0.25, \quad \frac{\gamma_1}{\gamma_0} = 2, \quad k_y = \frac{2\pi}{3a_0}$$

(graph near Dirac Point)

4. References

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