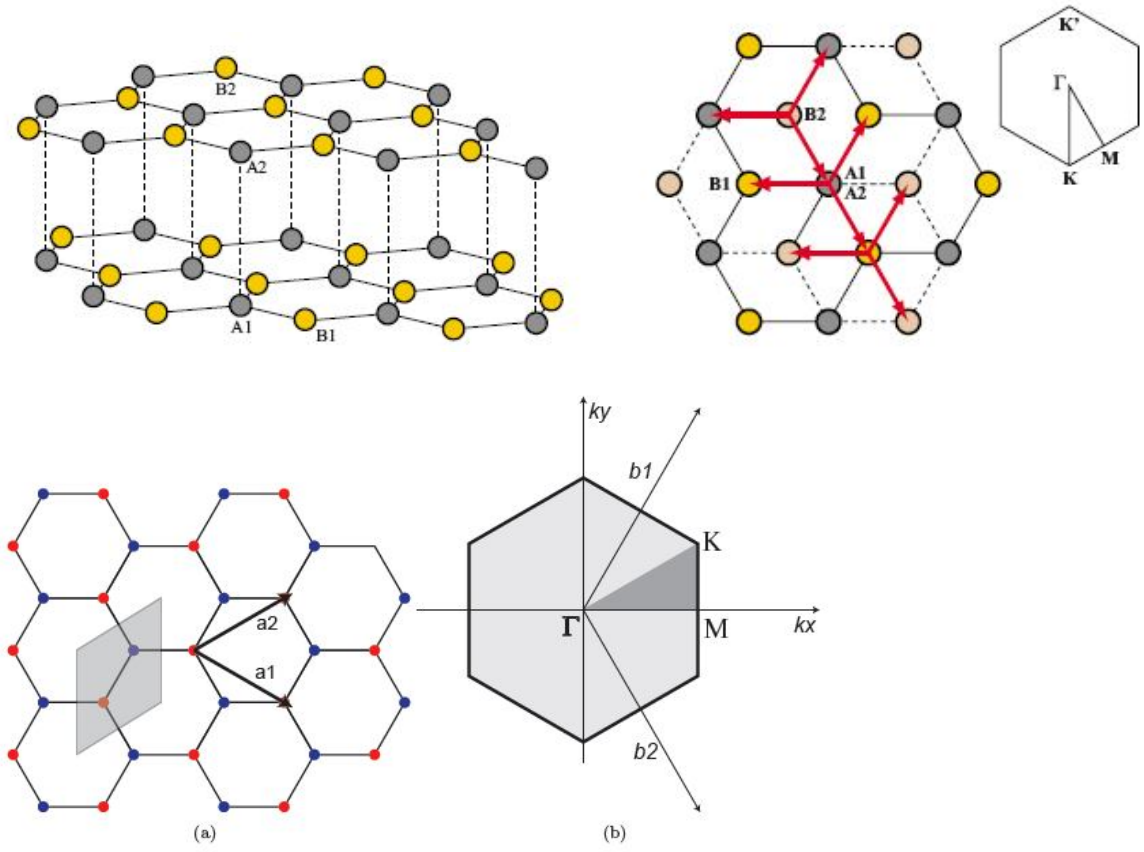
Tight Binding Based modelling of bilayer graphene

When electron is tightly bounded to nucleus, it is useful to express Hamiltonian in terms of one atom orbital creater and operator.

In case of bilayer graphene, we can construct bilayer graphene with two primitive lattice vectors and 4 atom basis, which we may call A1,B1,A2,B2. The lattice struce of graphene is shown below.



Here lattice vectors are given by

$$\mathrm{a}_1 = (\frac{\sqrt{3}}{2}, \frac{1}{2}, 0)a_0 \qquad \mathrm{a}_2 = (\frac{\sqrt{3}}{2}, -\frac{1}{2}, 0)a_0 \quad \text{where} \quad a_0 \quad \text{is lattice constant} \tag{1}$$

The nearest neighbor tight-binding Hamiltonian can be written as

$$\begin{aligned}\hat{H} &= -t\sum_{\mathbf{R}_i,\mathbf{r}_j}\left\{\hat{a}_1^+(\mathbf{R}_i^{A1})\hat{b}_1(\mathbf{R}_i^{A1}+\mathbf{r}_j)+\hat{a}_2^+(\mathbf{R}_i^{A2})\hat{b}_2(\mathbf{R}_i^{A2}+\mathbf{r}_j)+H.c\right\}\\ &\quad -\gamma\sum_{\mathbf{R}_i}\left\{\hat{a}_2^+(\mathbf{R}_i^{A1}+\mathbf{r}_4)\hat{a}_1(\mathbf{R}_i^{A1})+H.c\right\}\\ &\quad +\varepsilon\sum_{\mathbf{R}_i,j}\left\{\hat{a}_j^+(\mathbf{R}_i^{Aj})\hat{a}_j(\mathbf{R}_i^{Aj})+\hat{b}_j^+(\mathbf{R}_i^{Bj})\hat{b}_j(\mathbf{R}_i^{Bj})\right\}\\ \text{where } -t &= \left\langle\varphi,\vec{0}\middle|\hat{H}\middle|\varphi,\vec{0}+\mathbf{r}_i\right\rangle,\quad -\gamma=\left\langle\varphi,\vec{0}+\mathbf{r}_4\middle|\hat{H}\middle|\varphi,\vec{0}\right\rangle,\\ \varepsilon &= \left\langle\varphi,\vec{0}\middle|\hat{H}\middle|\varphi,\vec{0}\right\rangle\end{aligned} \tag{2}$$

Here $\hat{a}_j^+(\mathbf{R}_i^{Aj})$ is Aj atom orbital creator at $\mathbf{R}_i^{Aj}$ and $\hat{b}_j^+(\mathbf{R}_i^{Bj}+\mathbf{r}_i)$ is Bj atom orbital creator at the position of $\mathbf{R}_i^{Bj}+\mathbf{r}_i$. $|\varphi,\mathbf{R}\rangle$ is one atom π orbital centered on $\mathbf{R}$. $\mathbf{r}_i$ is the vector connecting the nearest neighbors which are given by

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

Using the Fourier transform

$$\hat{a}_j(\mathbf{R}_i^{Aj})=\int\frac{d^2k}{(2\pi)^2}e^{i\vec{k}\cdot\mathbf{R}_i^{Aj}}\hat{a}_j(\vec{k}),\quad \hat{b}_j(\mathbf{R}_i^{Bj})=\int\frac{d^2k}{(2\pi)^2}e^{i\vec{k}\cdot\mathbf{R}_i^{Bj}}\hat{b}_j(\vec{k}) \tag{4}$$

In (2) and set $\varepsilon=0$ result in

$$\begin{aligned}\hat{H} &= -t\sum_{\mathbf{R}_i,\mathbf{r}_j}\left\{\int\frac{d^2k'd^2k}{(2\pi)^4}e^{i(\vec{k}-\vec{k}')\cdot\mathbf{R}_i^{A1}}e^{i\vec{k}\cdot\mathbf{r}_j}\hat{a}_1^+(\vec{k}')\hat{b}_1(\vec{k})+\hat{a}_2^+\hat{b}_2\ \ term+H.c\right\}\\ &\quad -\gamma\sum_{\mathbf{R}_i}\left\{\int\frac{d^2k'd^2k}{(2\pi)^4}e^{i(\vec{k}-\vec{k}')\cdot\mathbf{R}_i^{A1}}e^{-i\vec{k}'\cdot\mathbf{r}_4}\hat{a}_2^+(\vec{k}')\hat{a}_1(\vec{k})+H.c\right\}\\ &= -t\sum_{\mathbf{r}_j}\left\{\int\frac{d^2k'd^2k}{(2\pi)^2}\left(\frac{1}{(2\pi)^2}\sum_{\mathbf{R}_i}e^{i(\vec{k}-\vec{k}')\cdot\mathbf{R}_i^{A1}}\right)e^{i\vec{k}\cdot\mathbf{r}_j}\hat{a}_1^+(\vec{k}')\hat{b}_1(\vec{k})+\hat{a}_2^+\hat{b}_2\ \ term+H.c\right\}\\ &\quad -\gamma\left\{\int\frac{d^2k'd^2k}{(2\pi)^4}\left(\frac{1}{(2\pi)^2}\sum_{\mathbf{R}_i}e^{i(\vec{k}-\vec{k}')\cdot\mathbf{R}_i^{A1}}\right)e^{-i\vec{k}'\cdot\mathbf{r}_4}\hat{a}_2^+(\vec{k}')\hat{a}_1(\vec{k})+H.c\right\}\end{aligned}$$

$$= -t\sum_{\mathbf{r}_j}\left\{\int\frac{d^2k}{(2\pi)^2}e^{i\vec{k}\cdot\mathbf{r}_j}\hat{a}_1^+(\vec{k})\hat{b}_1(\vec{k})+\hat{a}_2^+\hat{b}_2\ \ term+H.c\right\}$$

$$-\gamma\left\{\int\frac{d^2k}{(2\pi)^2}\hat{a}_2^+(\vec{k})\hat{a}_1(\vec{k})+H.c\right\}$$

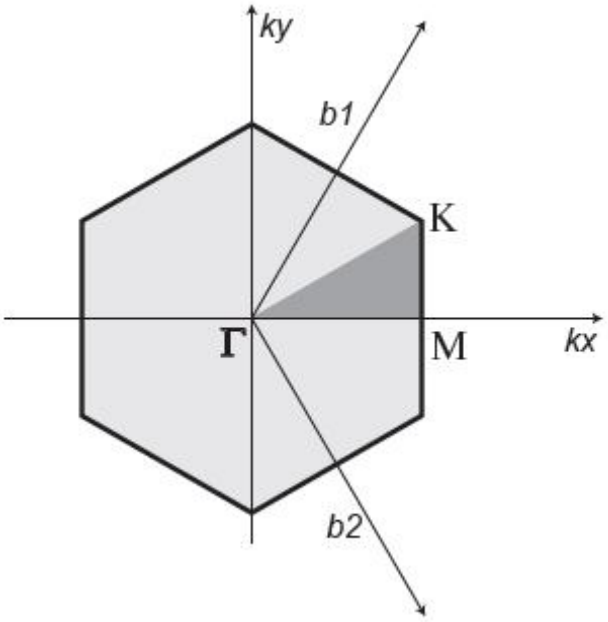
$$=\int\frac{d^2k}{(2\pi)^2}\begin{bmatrix}\hat{a}_1^+(\vec{k}) & \hat{b}_1^+(\vec{k}) & \hat{a}_2^+(\vec{k}) & \hat{b}_2^+(\vec{k})\end{bmatrix}\begin{bmatrix}0 & -t\cdot f(\vec{k}) & -\gamma & 0\\ -t\cdot f(\vec{k})^* & 0 & 0 & 0\\ -\gamma & 0 & 0 & -t\cdot f(\vec{k})\\ 0 & 0 & -t\cdot f(\vec{k})^* & 0\end{bmatrix}\begin{bmatrix}\hat{a}_1(\vec{k})\\ \hat{b}_1(\vec{k})\\ \hat{a}_2(\vec{k})\\ \hat{b}_2(\vec{k})\end{bmatrix}$$

where $f(\vec{k})=e^{i\vec{k}\cdot\mathbf{r}_1}+e^{i\vec{k}\cdot\mathbf{r}_2}+e^{i\vec{k}\cdot\mathbf{r}_3}=f_1(\mathbf{k})=e^{-ik_xa_0/\sqrt{3}}+2e^{ik_xa_0/(2\sqrt{3})}\cos(k_ya_0/2)$ (5)

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

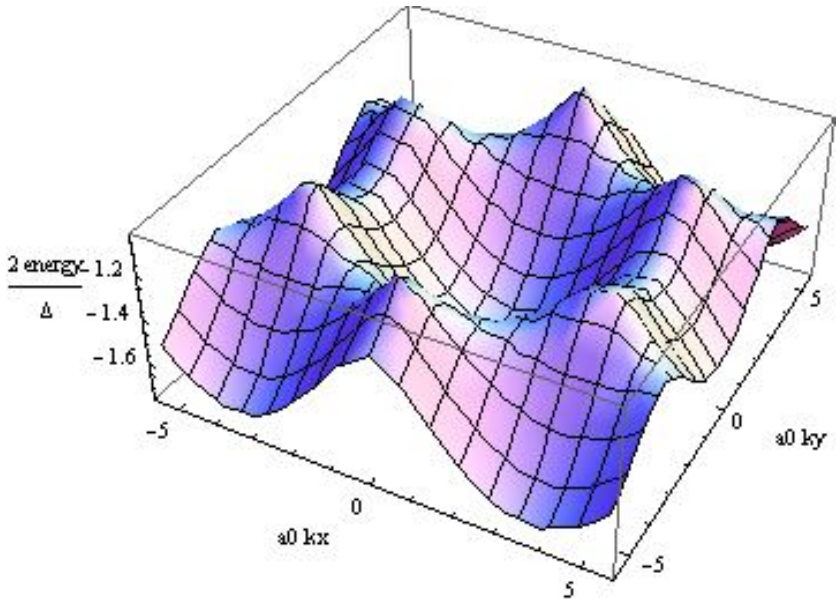
$$\mathbf{b}_1=(\frac{1}{\sqrt{3}},1)\frac{2\pi}{a_0},\quad \mathbf{b}_2=(\frac{1}{\sqrt{3}},-1)\frac{2\pi}{a_0} \tag{6}$$

From the reciprocal vectors the first Brillouin zone can be found. Below figure is describing Brillouin zone.

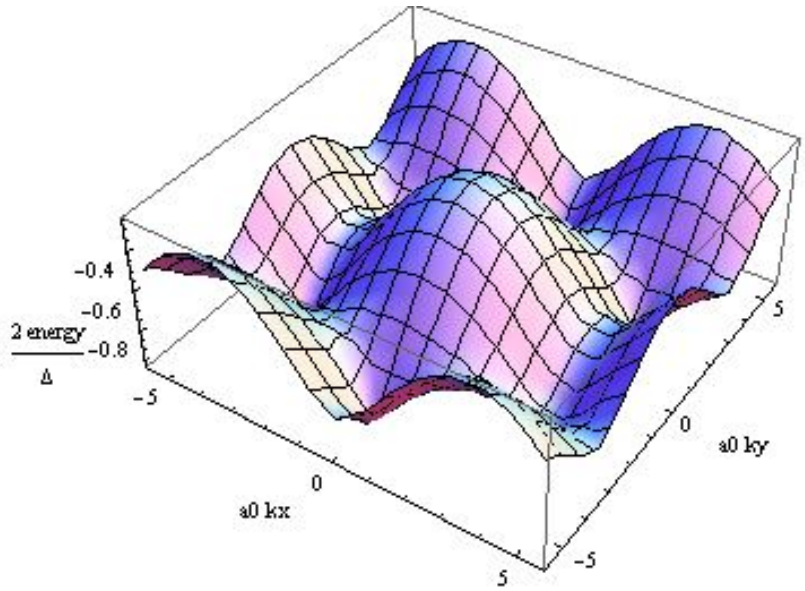


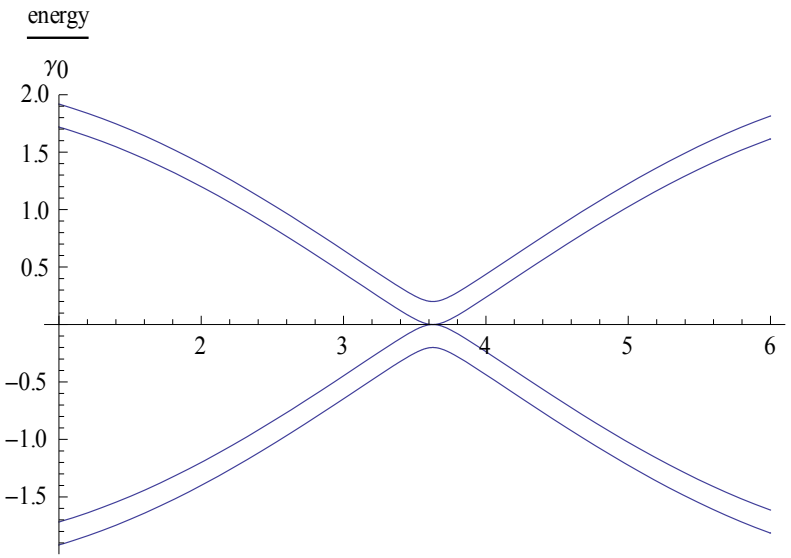
$K = (\frac{2\pi}{\sqrt{3}a_0}, \frac{2\pi}{3a_0})$ in the figure is called Dirac point.

Graph of band structure is like below.



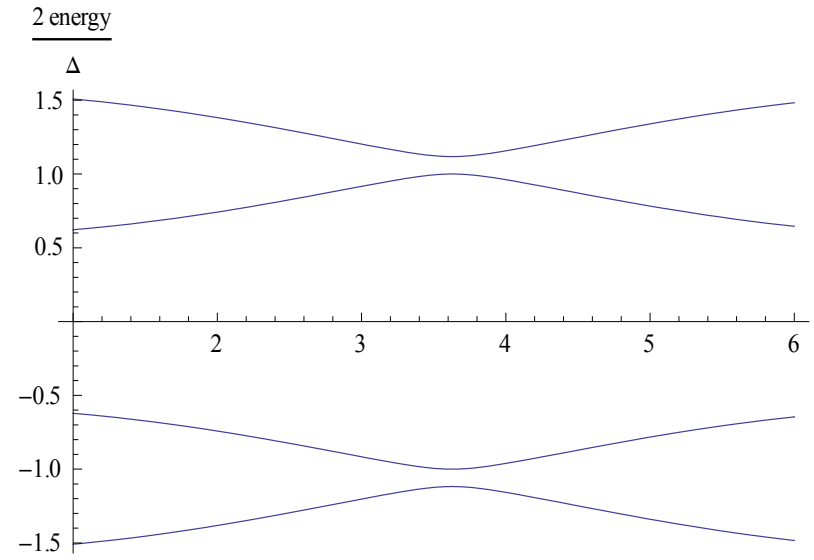
$\frac{t}{\Delta/2} = 0.25, \quad \frac{\gamma}{t} = 0.2$





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

(graph near Dirac Point)



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

(graph near Dirac Point)

References

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