The tight-binding model and low-energy effective model

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Outline

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What is tight binding model

Why band structure happens:

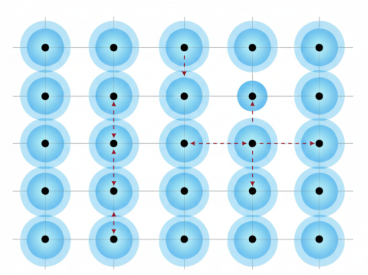
- The electrons of isolated atom occupy atomic orbitals with discrete energy levels
- If two atoms come close enough $\rightarrow$ their atomic orbitlas overlap $\rightarrow$ electrons can tunnel between the atoms
- This tunneling splits the atomic orbitals into molecular orbitals with different energies
- If a large number N of identical atoms come together to form a solid $\rightarrow$ Each discrete energy level splits into N levels, each with different energy

$$N \sim 10^{22}$$

- The adjacent levels are very closely spaced in energy $\rightarrow$ it can be considered to form a continuum (energy band)

What is tight binding model

- An approach to calculate band structure in solids
- The name "tight binding" suggests that the model describes the properties of tightly bound electrons in solids
- The electrons should have limited interaction with states on surrouding atoms of the solid



Why tight binding model

- When the number of atoms/electrons is very small $(N < 10) \rightarrow$ exact method

Calculations resource increase exponentially as N increases. And it become impossible

- $N <$ a few thousand atoms $\rightarrow$ density functional theory techinques
- $N > 10000 \rightarrow$ self-consistent DFT calculation is also impossible

Linear combination of atomic orbitals

$$H(\boldsymbol{r}) = H_{\text{at}}(\boldsymbol{r}) + \sum_{n \neq 0} V(\boldsymbol{r} - \boldsymbol{R}_n) = H_{\text{at}}(\boldsymbol{r}) + \Delta U(\boldsymbol{r})$$

Schrödinger equation

$$H\psi_m(\boldsymbol{r}) = \varepsilon_m \psi_m(\boldsymbol{r}) \leftarrow \text{Difficult to solve}$$

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- $V(\boldsymbol{r} - \boldsymbol{R}_n)$: atomic potentials at site $\boldsymbol{R}_n$
- ΔU is small enough
- Atomic orbitals $\varphi_m(\boldsymbol{r})$ are eigenstates of $H_{\mathsf{at}}(\boldsymbol{r})$

$$H_{\mathsf{at}}\varphi(\boldsymbol{r}) = \varepsilon_m \varphi_m(\boldsymbol{r})$$

- Linear combination of atomic orbitals (LCAO)

$$\psi_m(\boldsymbol{r}) = \sum_n b_m(\boldsymbol{R}_n)\varphi_m(\boldsymbol{r} - \boldsymbol{R}_n)$$

Bloch band

The Bloch theorem

$$\psi(\boldsymbol{r} + \boldsymbol{R}_l) = e^{i\boldsymbol{k}\cdot\boldsymbol{R}_l}\psi(\boldsymbol{r})$$

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$$\sum_n b_m(\boldsymbol{R}_n)\varphi_m(\boldsymbol{r} - (\boldsymbol{R}_n - \boldsymbol{R}_l)) = e^{i\boldsymbol{k}\cdot\boldsymbol{R}_l}\sum_n b_m(\boldsymbol{R}_n)\varphi_m(\boldsymbol{r} - \boldsymbol{R}_n)$$

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$$\sum_p b_m(\boldsymbol{R}_p + \boldsymbol{R}_l)\varphi_m(\boldsymbol{r} - \boldsymbol{R}_p) = e^{i\boldsymbol{k}\cdot\boldsymbol{R}_l}\sum_n b_m(\boldsymbol{R}_n)\varphi_m(\boldsymbol{r} - \boldsymbol{R}_n)$$

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$$\sum_n b_m(\boldsymbol{R}_n+\boldsymbol{R}_l)\varphi_m(\boldsymbol{r}-\boldsymbol{R}_n) = e^{i\boldsymbol{k}\cdot\boldsymbol{R}_l}\sum_n b_m(\boldsymbol{R}_n)\varphi_m(\boldsymbol{r}-\boldsymbol{R}_n)$$

Consequently

$$b_m(\boldsymbol{R}_n+\boldsymbol{R}_l) = e^{i\boldsymbol{k}\cdot\boldsymbol{R}_l}b_m(\boldsymbol{R}_n)$$

Tight-binding method

$$b_m(\boldsymbol{R}_n + \boldsymbol{R}_l) = e^{i\boldsymbol{k}\cdot\boldsymbol{R}_l} b_m(\boldsymbol{R}_n)$$

- $\boldsymbol{R}_n = 0 \rightarrow b_m(\boldsymbol{R}_l) = e^{i\boldsymbol{k}\cdot\boldsymbol{R}_l} b_m(0)$
- Normalization condition

$$\begin{aligned}
1 = \int \mathrm{d}\boldsymbol{r}\, \psi_m^*(\boldsymbol{r})\psi_m(\boldsymbol{r}) &= \sum_{n,l} \int \mathrm{d}\boldsymbol{r} b_m^*(0) e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_n} b_m(0) e^{i\boldsymbol{r}\cdot\boldsymbol{R}_l} \varphi_m^*(\boldsymbol{r} - \boldsymbol{R}_n)\varphi_m(\boldsymbol{r} - \boldsymbol{R}_l) \\
&= \sum_{n,l} e^{-i\boldsymbol{k}\cdot(\boldsymbol{R}_n - \boldsymbol{R}_l)} b_m^*(0) b_m(0) \int \mathrm{d}\boldsymbol{r}\, \varphi_m^*(\boldsymbol{r} - \boldsymbol{R}_n)\varphi_m(\boldsymbol{r} - \boldsymbol{R}_l) \\
&= \sum_{l} \sum_{p} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_p} b_m^*(0) b_m(0) \int \mathrm{d}\boldsymbol{x}\, \varphi_m^*(\boldsymbol{x} - \boldsymbol{R}_p)\varphi_m(\boldsymbol{x}) \\
&= N \sum_{p} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_p} b_m^*(0) b_m(0) \int \mathrm{d}x\, \varphi_m^*(\boldsymbol{x} - \boldsymbol{R}_p)\varphi_m(\boldsymbol{x})
\end{aligned}$$

In the above derivation, we set $\boldsymbol{x} = \boldsymbol{r} - \boldsymbol{R}_l$.

Tight-binding method

$$1 = N b_m^*(0) b_m(0) + N \sum_{p \neq 0} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_p} b_m^*(0) b_m(0) \int \mathrm{d}x \, \varphi_m^*(\boldsymbol{x} - \boldsymbol{R}_p) \varphi_m(\boldsymbol{x})$$

- Since we assume ΔU is small, the overlap of atomic orbitals can be safety neglected

And thus

$$b_m(0) \approx \frac{1}{\sqrt{N}}$$

and

$$\psi_m(\boldsymbol{r}) \approx \frac{1}{\sqrt{N}} \sum_n e^{i\boldsymbol{k}\cdot\boldsymbol{R}_n} \varphi_m(\boldsymbol{r} - \boldsymbol{R}_n)$$

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Outline

Band structure

Only consider the s-orbitals

$$\psi(\boldsymbol{r}) = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \phi_s(\boldsymbol{r} - \boldsymbol{R})$$

- Dispersion relation

$$\begin{aligned}
E(\boldsymbol{k}) &= \int \psi^*(\boldsymbol{r}) H \psi(\boldsymbol{r})\, \mathrm{d}\boldsymbol{r} \\
&= \frac{1}{N} \sum_{\boldsymbol{R},\boldsymbol{R}'} e^{i\boldsymbol{k}\cdot(\boldsymbol{R}'-\boldsymbol{R})} \int \mathrm{d}\boldsymbol{r}\, \phi_s^*(\boldsymbol{r}-\boldsymbol{R}) H \phi_s(\boldsymbol{r}-\boldsymbol{R}') \\
&= \frac{1}{N} \sum_{\boldsymbol{R},\boldsymbol{R}'} e^{i\boldsymbol{k}\cdot(\boldsymbol{R}'-\boldsymbol{R})} \int \mathrm{d}\boldsymbol{x}\, \phi_s^*(\boldsymbol{x}) H \phi_s(\boldsymbol{x}-(\boldsymbol{R}'-\boldsymbol{R})) \\
&= \sum_{\boldsymbol{R}''} e^{i\boldsymbol{k}\cdot\boldsymbol{R}''} \int \mathrm{d}\boldsymbol{x}\, \phi_s^*(\boldsymbol{x}) H \phi_s(\boldsymbol{x}-\boldsymbol{R}'') \\
&= \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \int \mathrm{d}\boldsymbol{x}\, \phi_s^*(\boldsymbol{x}) H \phi_s(\boldsymbol{x}-\boldsymbol{R})
\end{aligned}$$

Band structure

$$E(\boldsymbol{k}) = \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \int \mathrm{d}\boldsymbol{x}\, \phi_s^*(\boldsymbol{x}) H \phi_s(\boldsymbol{x} - \boldsymbol{R})$$

- $\boldsymbol{R}$ sums over all translation vector
- $\boldsymbol{R} = 0$ gives the s-orbital energy in isolated atom

$$\int \mathrm{d}\boldsymbol{x}\, \phi_s^*(\boldsymbol{x}) H \phi_s(\boldsymbol{x}) = \varepsilon_s$$

- Hopping energy

$$\sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} T(|\boldsymbol{R}|)$$

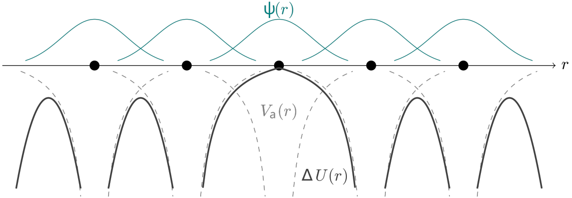
- For the s-orbital band

$$T(|\boldsymbol{R}|) = A e^{-\alpha R^2/R^2}$$

Single band in 1D crystal

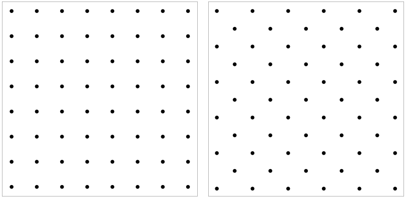
In a 1D crystal, the translation vectors $\boldsymbol{R} = n a_0 \hat{\mathbf{x}}$, where n is an integer

$$E(k) = \varepsilon_s + \left(e^{ika_0} + e^{-ika_0}\right) T(a_0) + \left(e^{2ika_0} + e^{-2ika_0}\right) T(2a_0) + \dots$$
$$\approx \varepsilon_0 + 2\cos(ka_0) T(a_0)$$



$T(2a_0)$ can be ignored since the overlap of the wavefunction in the next-nearest-neighbor is exponential small

Single band in $2D/3D$ crystal



With nearest hopping

$$E(k_x, k_y) = \varepsilon_s + 2T(a)\cos(k_x a) + 2T(b)\cos(k_y b)$$

N-atom basis

In a crystal with an N atom basis, the states can be expanded as combination of N Bloch states,

$$\psi_{m,\boldsymbol{k}}(\boldsymbol{r}) = \sum_i c_{i,\boldsymbol{k}} \phi_{i,\boldsymbol{k}}(\boldsymbol{r}) = \sum_i c_{i,\boldsymbol{k}} \frac{1}{\sqrt{N}} \sum_{\boldsymbol{R}_i} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_i} \phi(\boldsymbol{r} - \boldsymbol{R}_i)$$

The energy

$$\begin{aligned} E(\boldsymbol{k}) &= \sum_{i,j} c^*_{i,\boldsymbol{k}} c_{j,\boldsymbol{k}} \phi^*_{i,\boldsymbol{k}}(\boldsymbol{r}) H \phi_{j,\boldsymbol{k}}(\boldsymbol{r}) \\ &= \sum_{i,j} c^*_{i,\boldsymbol{k}} \langle \phi_{i,\boldsymbol{k}} | H | \phi_{j,\boldsymbol{k}} \rangle c_{j,\boldsymbol{k}} \\ &= \begin{pmatrix} c^*_{1,\boldsymbol{k}} & c^*_{2,\boldsymbol{k}} & \ldots \end{pmatrix} \langle \phi_{i,\boldsymbol{k}} | H | \phi_{j,\boldsymbol{k}} \rangle \begin{pmatrix} c_{1,\boldsymbol{k}} \\ c_{2,\boldsymbol{k}} \\ \vdots \end{pmatrix} \end{aligned}$$

We should find the lowest energy to determine the coefficient $c_{i,\boldsymbol{k}}$

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The Hamitonian is expanded in the basis of $\phi_{i,\boldsymbol{k}}(\boldsymbol{r})$

$$H_{ij} = \langle \phi_{i,\boldsymbol{k}} | H | \phi_{j,\boldsymbol{k}} \rangle$$

Finally, the energy structure can be determined by the eqaution

$$\det(H - E(\boldsymbol{k})I) = 0$$

Outline

Second quantization

$$\Psi(\boldsymbol{r}) = \sum_m a_m \psi_m(\boldsymbol{r}), \quad \psi_m(\boldsymbol{r}) = \sum_n b_m(\boldsymbol{R}_n)\varphi_m(\boldsymbol{r} - \boldsymbol{R}_n)$$

In second quantization, the basic object is the field operator

$$\Psi(\boldsymbol{r}) = \sum_{m,n} a_m b_m(\boldsymbol{R}_n)\varphi_m(\boldsymbol{r} - \boldsymbol{R}_n) \to \sum_{m,n} c_m(\boldsymbol{R}_n)\varphi_m(\boldsymbol{r} - \boldsymbol{R}_n)$$

Second quantization

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$$\hat{\Psi}(\boldsymbol{r}) = \sum_{m,n} \hat{c}_m(\boldsymbol{R}_n)\varphi_m(\boldsymbol{r} - \boldsymbol{R}_n)$$

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The Hamitonian in second quantization

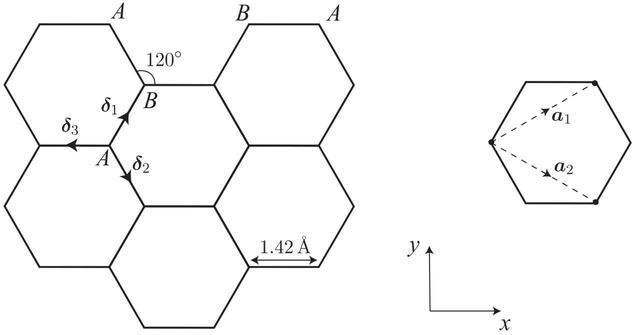
$$\begin{aligned}\hat{H} &= \int \mathrm{d}\boldsymbol{r}\, \hat{\Psi}^\dagger(\boldsymbol{r}) H \hat{\Psi}(\boldsymbol{r}) \\ &= \sum_{i,j,m} t_{ij}^{mn} c_m^\dagger(\boldsymbol{R}_i) c_n(\boldsymbol{R}_j)\end{aligned}$$

The hopping coefficient

$$t_{ij}^{mn} = \int \mathrm{d}\boldsymbol{r}\, \varphi_m^*(\boldsymbol{r} - \boldsymbol{R}_i) H \varphi_n(\boldsymbol{r} - \boldsymbol{R}_j)$$

Outline

Tight-binding model in single layer graphene



From Leggett's lecture

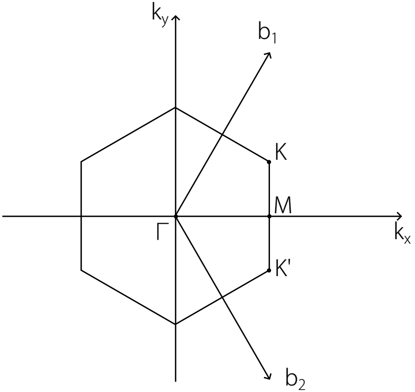
$$\boldsymbol{a}_1 = \frac{a}{2}\left(3, \sqrt{3}\right), \quad \boldsymbol{a}_2 = \frac{a}{2}\left(3, -\sqrt{3}\right)$$

The reciprocal lattice vectors $\boldsymbol{b}_1$, $\boldsymbol{b}_2$ defined by $\boldsymbol{a}_i \cdot \boldsymbol{b}_j = 2\pi\delta_{ij}$:

$$\boldsymbol{b}_1 = \frac{2\pi}{3a}\left(1, \sqrt{3}\right), \quad \boldsymbol{b}_2 = \frac{2\pi}{3a}\left(1, -\sqrt{3}\right)$$

Tight-binding model in single layer graphene

First Brillouin zone



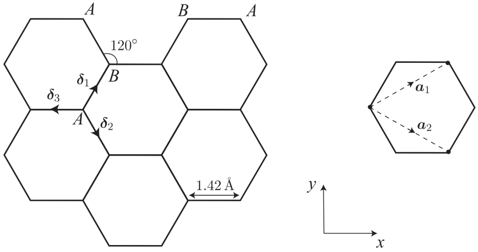
$$\boldsymbol{K} = \frac{2\pi}{3a}\left(1, \frac{1}{\sqrt{3}}\right), \quad \boldsymbol{K}' = \frac{2\pi}{3a}\left(1, -\frac{1}{\sqrt{3}}\right), \quad \boldsymbol{M} = \frac{2\pi}{3a}(1, 0)$$

- The electrons outside Carbon atom: $1\mathrm{s}^2 2\mathrm{s}^2 2\mathrm{p}^2$

Tight-binding model in single layer graphene

Only nearest neighbor hopping is considered

$$H = -t \sum_{\langle ij \rangle} \left(a_i^\dagger b_j + b_j^\dagger a_i \right) = -t \sum_{i \in A} \sum_{\boldsymbol{\delta}} \left(a_i^\dagger b_{i+\boldsymbol{\delta}} + b_{i+\boldsymbol{\delta}}^\dagger a_i \right)$$



$$\boldsymbol{\delta}_1 = \frac{a}{2}\left(1, \sqrt{3}\right), \quad \boldsymbol{\delta}_2 = \frac{a}{2}\left(1, -\sqrt{3}\right), \quad \boldsymbol{\delta}_3 = a\left(-1, 0\right)$$

Tight-binding model in single layer graphene

Fourier transform

$$a_i = \frac{1}{\sqrt{N/2}} \sum_{\boldsymbol{k}} e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_i} a_{\boldsymbol{k}}$$

where $N/2$ is the number of A sites.

$$\begin{aligned} H &= -\frac{t}{N/2} \sum_{i\in A} \sum_{\boldsymbol{\delta},\boldsymbol{k},\boldsymbol{k}'} \left[e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}_i} e^{-i\boldsymbol{k}'\cdot\boldsymbol{\delta}} a_k^\dagger b_{\boldsymbol{k}'} + \mathrm{H.\,c.} \right] \\ &= -t \sum_{\boldsymbol{\delta},\boldsymbol{k}} \left(e^{-i\boldsymbol{k}\cdot\boldsymbol{\delta}} a_{\boldsymbol{k}}^\dagger b_{\boldsymbol{k}} + \mathrm{H.\,c.} \right) \\ &= \begin{pmatrix} a_{\boldsymbol{k}} \\ b_{\boldsymbol{k}} \end{pmatrix}^\dagger \begin{pmatrix} 0 & \Delta_{\boldsymbol{k}} \\ \Delta_{\boldsymbol{k}}^* & 0 \end{pmatrix} \begin{pmatrix} a_{\boldsymbol{k}} \\ b_{\boldsymbol{k}} \end{pmatrix} \\ &= -t \sum_{\boldsymbol{\delta}} \left[\cos(\boldsymbol{k}\cdot\boldsymbol{\delta})\sigma_1 - \sin(\boldsymbol{k}\cdot\boldsymbol{\delta})\sigma_2 \right] \end{aligned}$$

Tight-binding model in single layer graphene

$$\begin{aligned}\Delta_{\boldsymbol{k}} &= e^{i\boldsymbol{k}\cdot\boldsymbol{\delta}_1} + e^{i\boldsymbol{k}\cdot\boldsymbol{\delta}_2} + e^{i\boldsymbol{k}\cdot\delta_3} \\ &= e^{-ik_x a}\left[1 + 2e^{i3k_x a/2}\cos\left(\frac{\sqrt{3}}{2}k_y a\right)\right]\end{aligned}$$

The energy spectrum

$$\begin{aligned}E(\boldsymbol{k}) &= \pm t\sqrt{\Delta_{\boldsymbol{k}}\Delta_{\boldsymbol{k}}^*} \\ &= \pm t\sqrt{1 + 4\cos\left(\frac{3}{2}k_x a\right)\cos\left(\frac{\sqrt{3}}{2}k_y a\right) + 4\cos^2\left(\frac{\sqrt{3}}{2}k_y a\right)}\end{aligned}$$

- For $\boldsymbol{k} = \boldsymbol{K}$ or $\boldsymbol{K}'$, $\Delta_{\boldsymbol{k}} = 0$, gapless bands

Tight-binding model in single layer graphene

$$\Delta_{\boldsymbol{K}+\boldsymbol{q}} \approx \Delta(\boldsymbol{K}) + \left.\frac{\partial \Delta_{\boldsymbol{k}}}{\partial \boldsymbol{k}}\right|_{\boldsymbol{k}=\boldsymbol{K}} \boldsymbol{q} = -ie^{-iK_x a}\frac{3a}{2}\left(q_x + iq_y\right)$$

Near the Dirac point $\boldsymbol{K}$, the Hamiltonian is thus

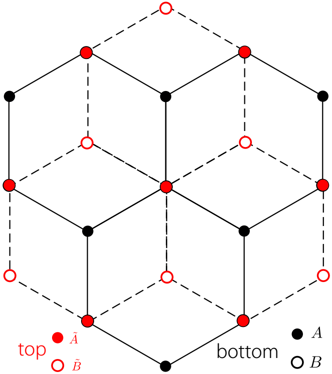
$$H(\boldsymbol{K}+\boldsymbol{q}) = v_F \begin{pmatrix} 0 & q_x + iq_y \\ q_x - iq_y & 0 \end{pmatrix} = v_F\left(q_x\sigma_1 - q_y\sigma_2\right)$$

Near $\boldsymbol{K}'$

$$H(\boldsymbol{K}'+\boldsymbol{q}) = v_F \begin{pmatrix} 0 & q_x - iq_y \\ q_x + iq_y & 0 \end{pmatrix} = v_F\left(q_x\sigma_1 + q_y\sigma_2\right)$$

Effective model in bilayer graphene

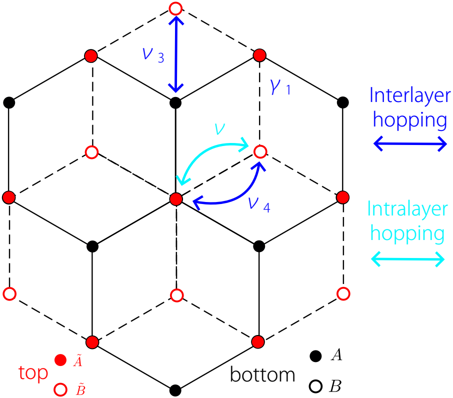
AB-stacking



- Bernal type
- One A atom in the top layer ($\tilde{A}$) lies above a B atom in the bottom layer

Effective model in bilayer graphene

AB-stacking



- Bernal type
- One A atom in the top layer ($\tilde{A}$) lies above a B atom in the bottom layer

Effective model in bilayer graphene

$$H = \begin{array}{cc} & \begin{array}{cccc} A & \tilde{B} & \tilde{A} & B \end{array} \\ & \begin{pmatrix} 0 & 0 & 0 & \nu\pi^\dagger \\ 0 & 0 & \nu\pi & 0 \\ 0 & \nu\pi^\dagger & 0 & 0 \\ \nu\pi & 0 & 0 & 0 \end{pmatrix} \begin{array}{c} A \\ \tilde{B} \\ \tilde{A} \\ B \end{array} \end{array}$$

where $\pi^\dagger = k_x - ik_y$

- No any inter-layer coupling

Effective model in bilayer graphene

$$
\begin{array}{c c}
\begin{array}{cccc} A & \tilde{B} & \tilde{A} & B \end{array} & \\
H = \begin{pmatrix} 0 & 0 & 0 & \nu\pi^\dagger \\ 0 & 0 & \nu\pi & 0 \\ 0 & \nu\pi^\dagger & 0 & \gamma_1 \\ \nu\pi & 0 & \gamma_1 & 0 \end{pmatrix} & \begin{array}{c} A \\ \tilde{B} \\ \tilde{A} \\ B \end{array}
\end{array}
$$

where $\pi^\dagger = k_x - ik_y$

- Coupling between $\tilde{A}$ and B

Effective model in bilayer graphene

$$H = \begin{array}{c} \\ \\ \\ \\ \\ \end{array}\begin{array}{cc} \begin{array}{cccc} \quad A & \quad \tilde{B} & \quad \tilde{A} & \quad B \end{array} & \\ \begin{pmatrix} 0 & \nu_3\pi & 0 & \nu\pi^\dagger \\ \nu_3\pi^\dagger & 0 & \nu\pi & 0 \\ 0 & \nu\pi^\dagger & 0 & \gamma_1 \\ \nu\pi & 0 & \gamma_1 & 0 \end{pmatrix} & \begin{array}{c} A \\ \tilde{B} \\ \tilde{A} \\ B \end{array} \end{array}$$

where $\pi^\dagger = k_x - ik_y$

- Coupling between $\tilde{A}$ and B
- Coupling between A and $\tilde{B}$

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Effective model in bilayer graphene

$$H = \begin{array}{cc} \begin{matrix} \quad A & \quad \tilde{B} & \quad \tilde{A} & \quad B \end{matrix} & \\ \begin{pmatrix} 0 & \nu_3 \pi & \nu_4 \pi^\dagger & \nu \pi^\dagger \\ \nu_3 \pi^\dagger & 0 & \nu \pi & \nu_4 \pi \\ \nu_4 \pi & \nu \pi^\dagger & 0 & \gamma_1 \\ \nu \pi & \nu_4 \pi^\dagger & \gamma_1 & 0 \end{pmatrix} & \begin{matrix} A \\ \tilde{B} \\ \tilde{A} \\ B \end{matrix} \end{array}$$

where $\pi^\dagger = k_x - i k_y$

- Coupling between $\tilde{A}$ and B
- Coupling between A and $\tilde{B}$
- Coupling between A/B and $\tilde{A}/\tilde{B}$

$$v = 8 \times 10^5\ \mathrm{m/s},\ \gamma_1 = 0.39\,\mathrm{eV}$$

Outline

Summary

- Tight-binding model
- Calculate the band spectrum: Band width, band gap
- Surface states, many-body problem and quasiparticle calculations