Tight Binding Approximation

Hasdeo

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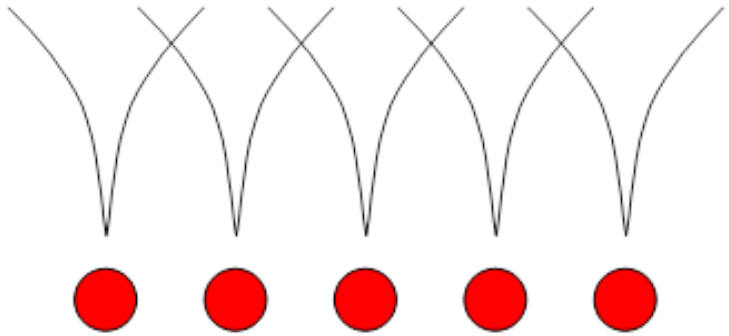
Outline

1. 1D chain 2 kinds of atom
2. 2D 2 kinds of atom
3. Computer Excercise

Prosedur Mendapatkan Dispersi Energi

1. Tentukan
   1. unit cell dan unit vektor $\mathbf{a}_i$,
   2. tentukan koordinat atom pada unit cell
   3. dan tentukan jumlah n orbital atom yang diperhitungkan
2. Carilah Brillouin zone dan reciprocal lattice vector $\mathbf{b}_i$
3. Hitung $\mathscr{H}_{ij}(\mathbf{k})$ dan $S_{ij}(\mathbf{k})$
4. Selesaikan persamaan sekular, dapatkan $E_i(\mathbf{k})$ dan $C_{ij}(\mathbf{k})$.

Contoh Rantai Metal 1D



Diketahui:

1. satu atom per unit cell, $\mathbf{a}_i = a\hat{\mathbf{x}}$, jumlah orbital = 1

$$\Psi_k(x) = \frac{1}{\sqrt{N}} \sum_{l=1}^{N} e^{ikla} \psi(x - la) \tag{1}$$

2. Hamiltonian

$$\mathscr{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(x)$$

Contoh Rantai Metal 1D

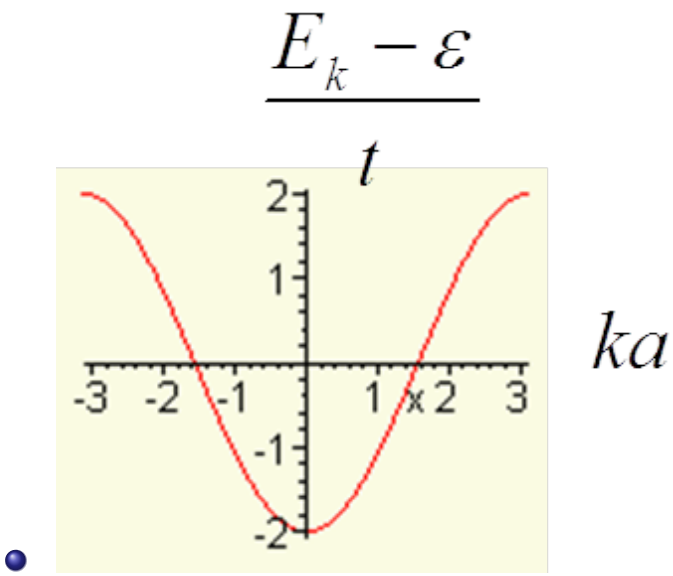
- Dispersi energi

$$
\begin{aligned}
E_k(\mathbf{k}) &= \frac{\langle \Psi_k | \mathscr{H} | \Psi_k \rangle}{\langle \Psi_k | \Psi_k \rangle} && (2)\\
&= \frac{\frac{1}{N}\sum_{l,m=1}^{N} e^{ik(m-l)a} \int dx\, \psi^*(x-la)\, \mathscr{H}\, \psi(x-ma)}{\frac{1}{N}\sum_{l,m=1}^{N} e^{ik(m-l)a} \int dx\, \psi^*(x-la)\, \psi(x-ma)} && (3)\\
&= \frac{\sum_{l,m=1}^{N} e^{ik(m-l)a}\, \mathscr{H}_{lm}}{\sum_{l,m=1}^{N} e^{ik(m-l)a} S_{lm}} && (4)
\end{aligned}
$$

Contoh Rantai Metal 1D

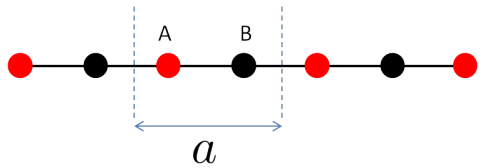
- Aproksimasi 1 tetangga terdekat,

$$E_j(\mathbf{k}) = \frac{H_0 + e^{ika}H_1 + e^{-ika}H_1}{S_0}$$
$$E_j(\mathbf{k}) = \varepsilon - t\cos(ka)$$

- 

- Kerjakan soal yang sama untuk bila atom A dan B saling bergantian dengan transfer integral t_1 dan t_2.

1D chain 2 kinds of atom



1. 2 atoms per unit cell $\rightarrow$ hamiltonian H dan overlap matrix S 2x2 matrix

$$\{H\} = \begin{pmatrix} H_{\mathrm{AA}} & H_{\mathrm{AB}} \\ H_{\mathrm{BA}} & H_{,\mathrm{BB}} \end{pmatrix}, \{S\} = \begin{pmatrix} S_{\mathrm{AA}} & S_{\mathrm{AB}} \\ S_{\mathrm{BA}} & S_{,\mathrm{BB}} \end{pmatrix}$$

2. Assumption

$$\begin{aligned} H_{\mathrm{AA}} &= -H_{\mathrm{BB}} = \Delta \\ H_{\mathrm{AB}} &= t_1 e^{ika/2} + t_2 e^{-ika/2} \\ H_{\mathrm{BA}} &= H^*_{\mathrm{AB}} \\ S_{ij} &= \delta_{ij} \end{aligned}$$

1D chain 2 kinds of atom

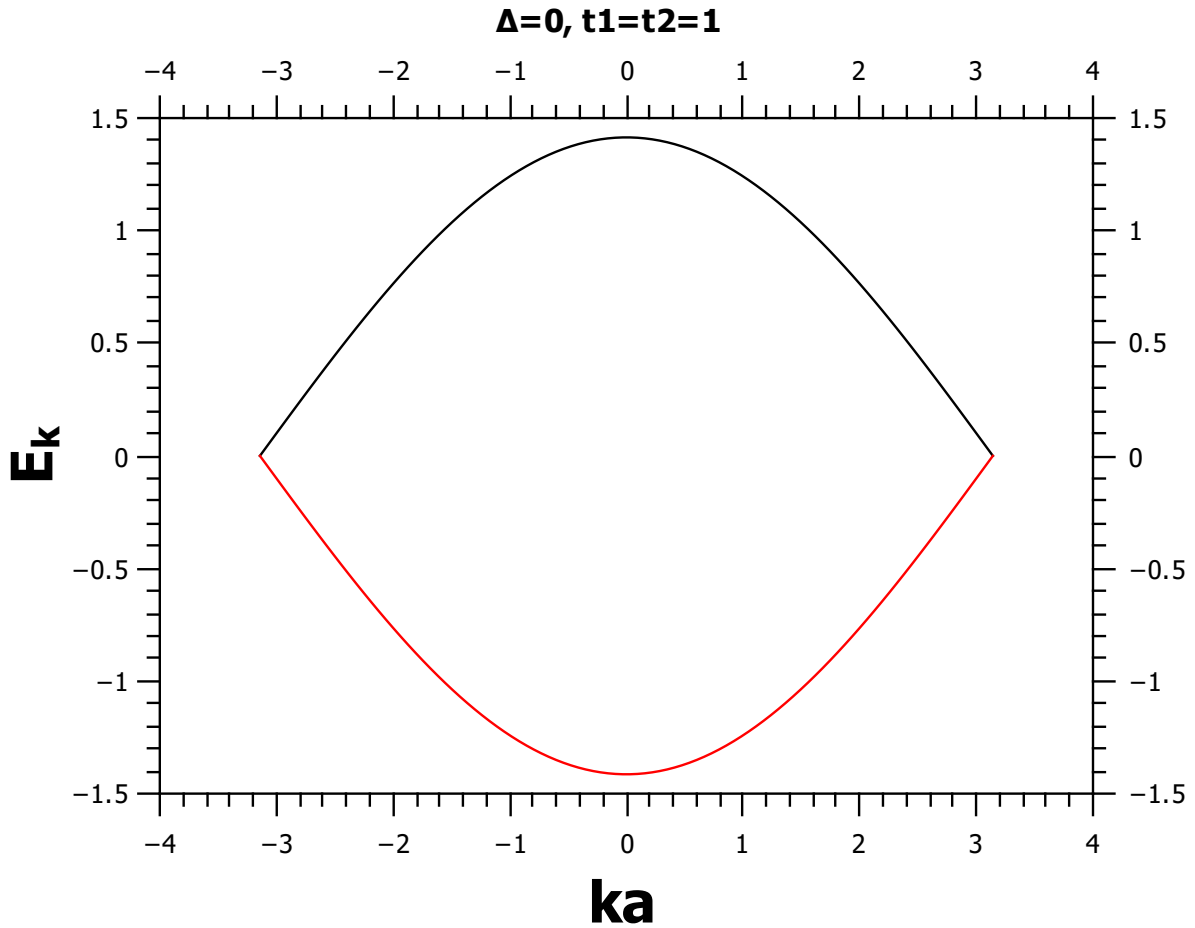
1. Persamaan Sekular

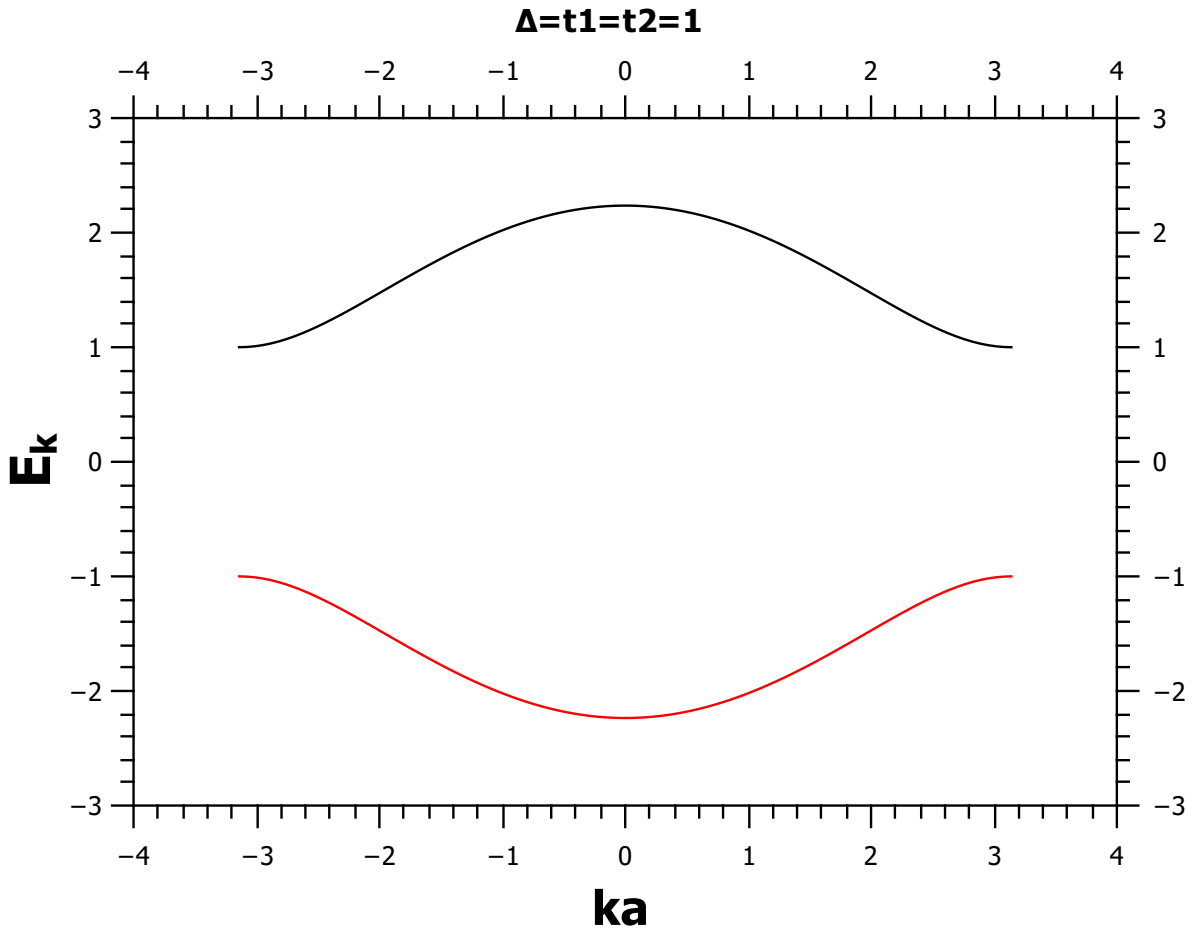
$$\det\left[H - E_k S\right] = 0$$

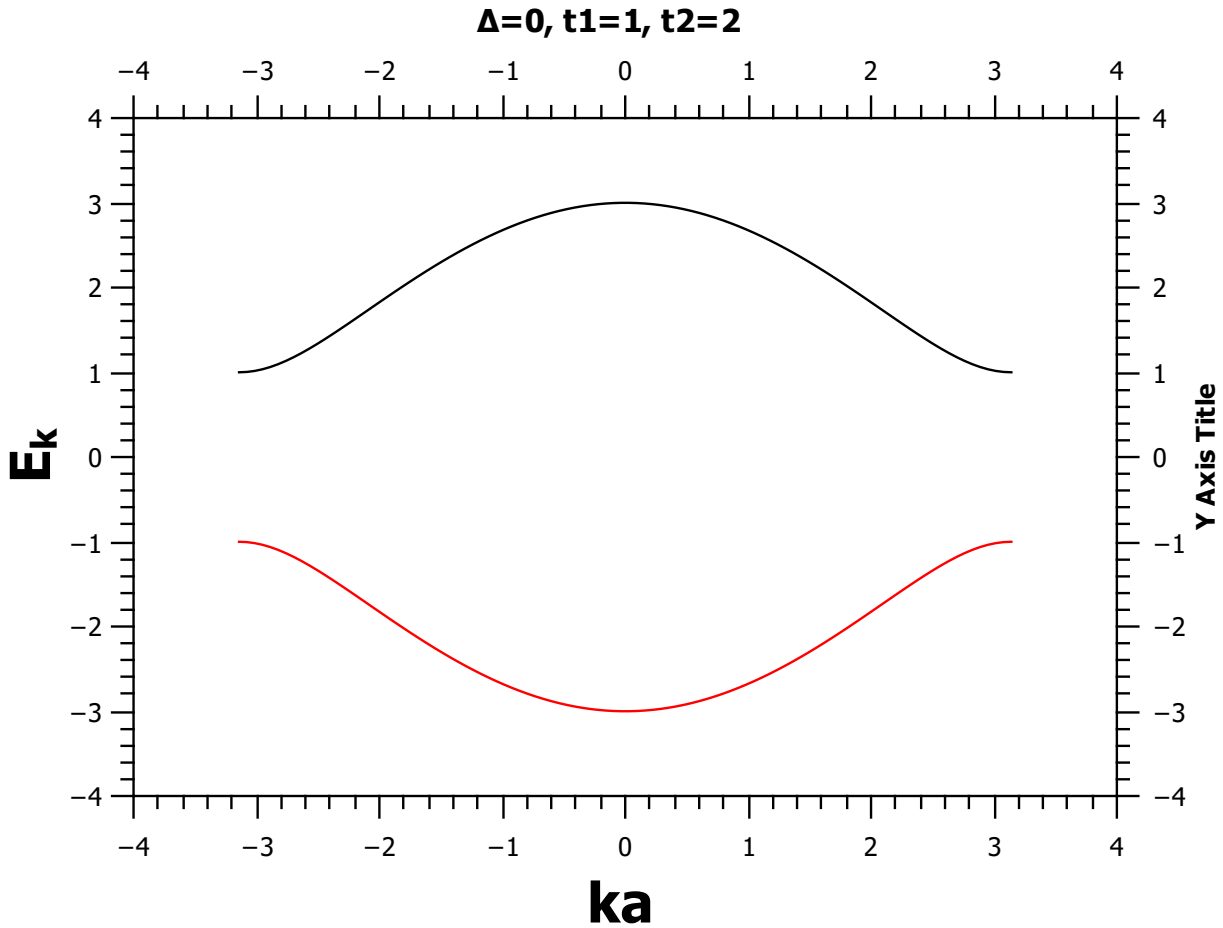
$$\det\begin{bmatrix} \Delta - E_k & t_1 e^{ika/2} + t_2 e^{-ika/2} \\ t_1 e^{-ika/2} + t_2 e^{ika/2} & -\Delta - E_k \end{bmatrix} = 0$$

2. Dispersi energy

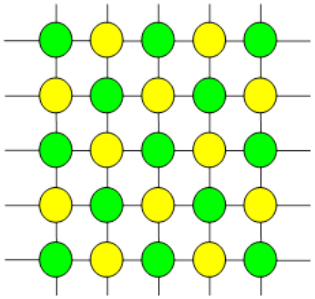
$$E_k = \pm\sqrt{\Delta^2 + t_1^2 + t_2^2 + 2t_1 t_2 \cos\left(ka\right)}$$


Δ=0, t1=t2=1
Ek
ka
−4
−3
−2
−1
0
1
2
3
4
1.5
1
0.5
0
−0.5
−1
−1.5


Δ=t1=t2=1
Ek
ka
−4
−3
−2
−1
0
1
2
3
4


Δ=0, t1=1, t2=2
Ek
ka
Y Axis Title
−4 −3 −2 −1 0 1 2 3 4

2D 2 kinds of atom



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2. Assumption

$$\begin{aligned} H_{\mathrm{AA}} &= -H_{\mathrm{BB}} = \Delta \\ H_{\mathrm{AB}} &= t\left(e^{ik_x a/2} + e^{-ik_x a/2} + e^{ik_y a/2} + e^{-ik_y a/2}\right) \\ H_{\mathrm{BA}} &= H^*_{\mathrm{AB}} \\ S_{ij} &= \delta_{ij} \end{aligned}$$

Bagaimana dengan dispersi energinya?

Install Fortran

Let's learn how to install Fortran and Compile it.