TIGHT-BINDING METHOD
UNTUK KOMPUTASI STRUKTUR ELEKTRONIK

Quantum Matter Theory's MBKM TEAM
Research Center for Quantum Physics

BRIN
BADAN RISET
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Silabus dan Penyetaraan SKS

No	Kompetensi Teknis	SKS
1.	Teori Optika Kuantum	4
2.	Metode Komputasi Mekanika Kuantum	2
3.	Komputasi Material dan Spektroskopi	2
4.	Pengolahan dan Visualisasi Data	3
5.	Pelaksanaan Proyek Riset	2
6.	Penulisan Laporan Riset	2
7.	Presentasi Riset	1
	Jumlah SKS	**16**

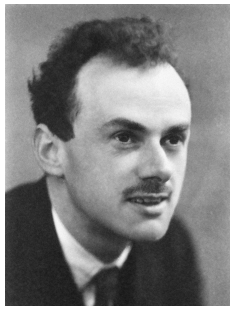
No	Kompetensi Manajerial	SKS
1.	Komunikasi	1
2.	Kerja Sama	1
3.	Tanggung Jawab	1
4.	Penyelesaian Masalah	1
	Jumlah SKS	**4**

Total SKS = Kompetensi Manajerial + Teknis = **20 SKS**

Rujukan utama:

(1) Gerry and Knight (2005), Introductory Quantum Optics, target minimal s.d. bab 4 terbahas
(2) Izaac and Wang (2018), Computational Quantum Mechanics, target paham Python + Fortran
(3) Hung, Nugraha, and Saito (2022), Quantum ESPRESSO Course for Solid State Physics, target s.d. epsilon.x
(4) QuasiTutorial: Modul Praktis untuk Riset Teori dan Komputasi Material, seluruh bab kecuali BoltzTraP
(5) QuTiP Tutorial @qutip.org, sesuai minat proyek yang akan dilakukan
(6) LaTeX Tutorial @overleaf.com dan The Not So Short Introduction to LaTeX

Teori kuantum sudah komplet?



Paul A. M. Dirac
Proc. R. Soc. Lond. A, 123, 714-733 (1929)

Quantum Mechanics of Many-Electron Systems.

By P. A. M. Dirac, St. John's College, Cambridge.

(Communicated by R. H. Fowler, F.R.S.—Received March 12, 1929.)

§ 1. *Introduction.*

The general theory of quantum mechanics is now almost complete, the imperfections that still remain being in connection with the exact fitting in of the theory with relativity ideas. These give rise to difficulties only when high-speed particles are involved, and are therefore of no importance in the consideration of atomic and molecular structure and ordinary chemical reactions, in which it is, indeed, usually sufficiently accurate if one neglects relativity variation of mass with velocity and assumes only Coulomb forces between the various electrons and atomic nuclei. The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble. It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation.

- **Hukum-hukum dasar** yang diperlukan untuk melakukan prosedur matematis dari **sebagian besar ilmu fisika** dan **seluruh ilmu kimia** telah diketahui sepenuhnya.
- **Kesulitan**nya hanya terletak pada kenyataan bahwa penerapan hukum-hukum ini sering memberikan **persamaan yang terlalu rumit untuk dipecahkan**.

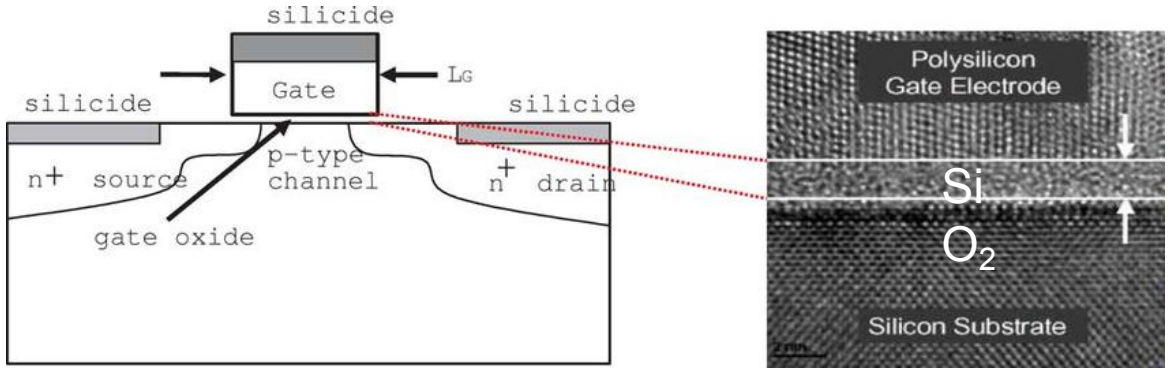
→ **Pentingnya metode komputasi yang tepat!**

Sains prediktif untuk sifat material

Ada beragam material dan aplikasinya yang dapat kita prediksi secara *bottom-up*

Material rangka

Bahan obat



Mikroelektronika/
Nanoelektronika

S. J. Bae et al., IEEE Trans Reliab. **56**, 392–400 (2007)

Tantangan kompleksitas

Fungsi gelombang elektron berada pada ruang berdimensi 3*n*

$$\psi(\{r_i\};\{R_i\})$$

Tinjau contoh kasus *unit* cell untuk kristal silikon (2 atom → 28 elektron)

Misalkan kita mau menghitung integral solusi persamaan Schrodinger, diskretisasi setiap dimensi derajat kebebasan elektron dengan 10 titik. Apa yang terjadi?

- Operasi perhitungan integral yang perlu dilakukan adalah $10^{(3x28)} = 10^{84}$
- Superkomputer canggih *exascale* bisa melakukan 10^{18} operasi per detik
- Berarti **kita butuh 10^{66} detik!** (padahal usia alam semesta "cuma" 10^{17} s)

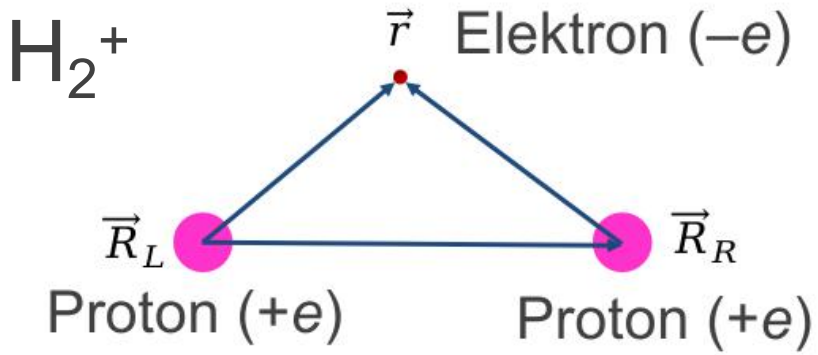
Urgensi Metode Aproksimasi

- **Aproksimasi ikatan terkuat (*tight-binding approximation*) / LCAO**
- Teori gangguan (*perturbation theory*)
- Metode variasi (*variational method*)
- ...

Cara lain: perumusan ulang mekanika kuantum

- Teori fungsional kerapatan (*density functional theory*)
- Formulasi ruang fase (*phase-space formulation of quantum mechanics*)
- ...

Molekul paling sederhana

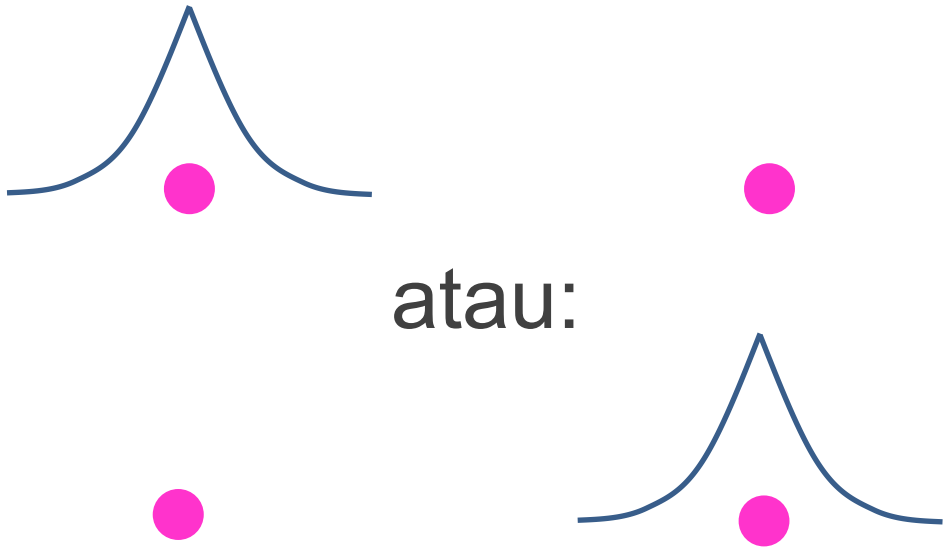


Hamiltonian Born-Oppenheimer:

$$H = -\frac{\hbar^2}{2m}\vec{\nabla}_r^2 - \frac{e^2}{|\vec{r}-\vec{R}_L|} - \frac{e^2}{|\vec{r}-\vec{R}_R|} + \frac{e^2}{|\vec{R}_R-\vec{R}_L|}$$

Fungsi gelombang H_2^+

Jika dua proton berjauhan:



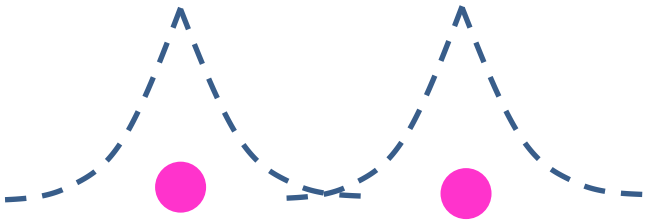
atau:

$$\psi_{1s}\left(\vec{r}-\vec{R}_L\right)=\psi_L$$

$$\psi_{1s}\left(\vec{r}-\vec{R}_R\right)=\psi_R$$

Orbital molekuler
Kombinasi linear orbital atomik (LCAO)

Jika dua proton berdekatan:



$$\psi_{\mathrm{MO}}=a_L\psi_L+a_R\psi_R$$

Linear Combination of Atomic Orbitals

Kombinasi linear orbital atom: $\Psi(x) = \sum_{i=1}^{N} C_i \varphi(x - \mathbf{R}_i)$

(*linear combination of atomic orbitals* / LCAO)

$\varphi(x - \mathbf{R}_i)$: Orbital atom pada $\mathbf{R} = \mathbf{R}_i$

Perhitungan energi:

$$E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{\sum_{i,j} C_i^* C_j H_{ij}}{\sum_{i,j} C_i^* C_j S_{ij}}$$

$S_{ij} = \langle \varphi_i | \varphi_j \rangle : \mathbf{S}$ (*Overlap matrix*)

$H_{ij} = \langle \varphi_i | H | \varphi_j \rangle : \mathbf{H}$ (*Hamiltonian matrix*)

$$\sum_j C_j H_{ij} - E \sum_j C_j S_{ij} = 0, (i = 1, \cdots, N)$$

Overlap matrix $\mathbf{S} = \{S_{ij}\}$, $\mathbf{C} = {}^{\mathrm{t}}\{C_j\}$

$(\mathbf{H} - E\mathbf{S})\mathbf{C} = 0$ Hamiltonian matrix $\mathbf{H} = \{H_{ij}\}$

$\mathbf{C} \neq 0 \Leftrightarrow \det(\mathbf{H} - E\mathbf{S}) = 0$

Secular equation

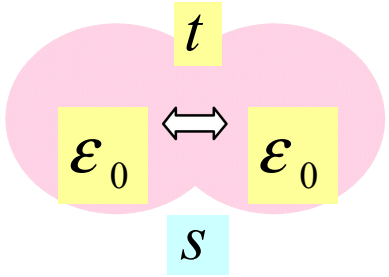
Langkah Perhitungan

- Isi matriks H dan S
- Pecahkan determinan persamaan sekuler
- Dapatkan nilai eigen dan vektor eigen
- Susun keadaan elektron dari energi terendah

Fungsi eigen dibentuk dari koefisien vektor eigen

$$\Psi_k(x) = \sum_{i=1}^{N} C_{ik}\varphi(x - \mathbf{R}_i)$$

Contoh molekul hidrogen: 2 elektron 2 orbital 1s



$$H = \begin{pmatrix} \varepsilon_0 & t \\ t & \varepsilon_0 \end{pmatrix}, \; S = \begin{pmatrix} 1 & s \\ s & 1 \end{pmatrix}$$

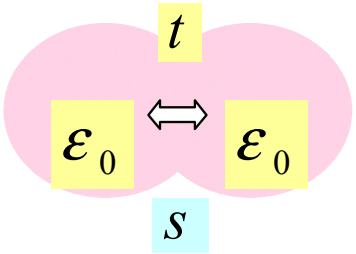
$$\Psi(x) = C_1\varphi_1 + C_2\varphi_2$$

$$\det(H - ES) = \begin{vmatrix} \varepsilon_0 - E & t - sE \\ t - sE & \varepsilon_0 - E \end{vmatrix} = 0$$

Hasil untuk molekul hidrogen

$$\det(H-ES)=\begin{vmatrix}\varepsilon_0-E & t-sE\\ t-sE & \varepsilon_0-E\end{vmatrix}=0$$

$t<0,\ s>0$

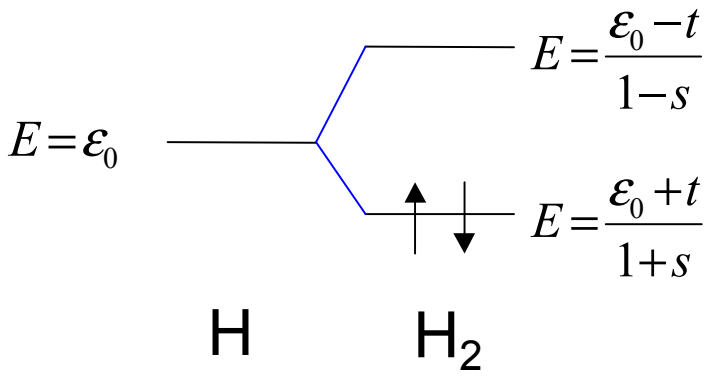


$$\Psi(x)=C_1\varphi_1+C_2\varphi_2$$

Energi: $E=\dfrac{\varepsilon_0\pm t}{1\pm s}$

Vektor eigen:

$$\begin{pmatrix}\varepsilon_0-E & t-sE\\ t-sE & \varepsilon_0-E\end{pmatrix}\begin{pmatrix}C_1\\ C_2\end{pmatrix}=0$$



Masukkan nilai setiap energi ke persamaan matriks

$$E=\frac{\varepsilon_0+t}{1+s}\ \Leftrightarrow\ C_1:C_2=1:1$$

$$E=\frac{\varepsilon_0-t}{1-s}\ \Leftrightarrow\ C_1:C_2=1:-1$$

Normalisasi

$$|\psi|^2=1\Leftrightarrow|C_1|^2+2|C_1||C_2|s+|C_2|^2=1$$

$$\begin{pmatrix}C_1\\ C_2\end{pmatrix}=\frac{1}{\sqrt{2(1+s)}}\begin{pmatrix}1\\ 1\end{pmatrix},\ \frac{1}{\sqrt{2(1-s)}}\begin{pmatrix}1\\ -1\end{pmatrix}$$

Molekul 3 atom?

Contoh: Li_3 (basis 3 elektron 2s)

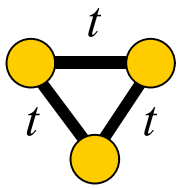
Aproksimasi $t < 0$ dan $s = 0$ **S** = **I** (matriks identitas)

- Rantai linear

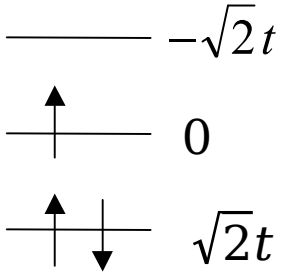
$$H = \begin{pmatrix} 0 & t & 0 \\ t & 0 & t \\ 0 & t & 0 \end{pmatrix}$$

- Segitiga

$$H = \begin{pmatrix} 0 & t & t \\ t & 0 & t \\ t & t & 0 \end{pmatrix}$$

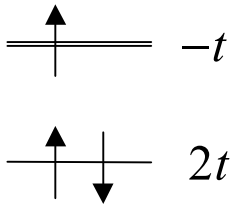


$$E = 0, \pm\sqrt{2}\,t \qquad \Leftarrow \det(H - EI) = 0 \Rightarrow \qquad E = 2t, -t, -t$$

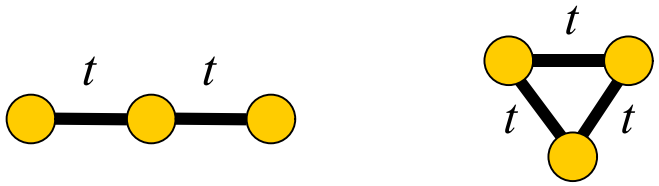


Manakah struktur yang lebih stabil?

Cari energi total yang lebih rendah!



Kuis



Asumsikan $t < 0$, konfigurasi paling stabil dari molekul Li_3 adalah:

(A) Rantai linear dengan energi total $2\sqrt{2}t$

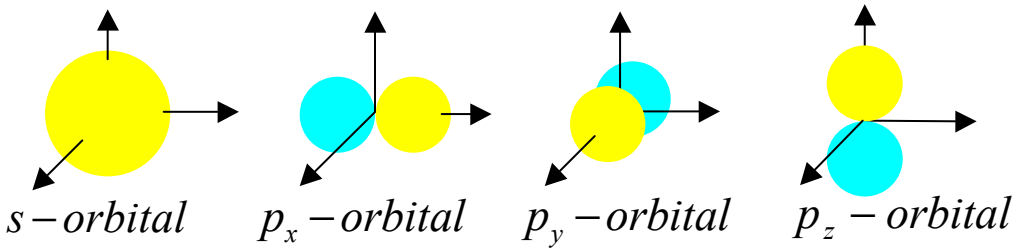
(B) Segitiga dengan energi total 0

(C) Segitiga dengan energi total $3t$

(D) Rantai linear dengan energi total $-\sqrt{2}t$

Lebih banyak orbital atom?

$$C: 1s^2, 2s^2, 2p^2$$



Contoh: C_2 Setiap atom menyumbang basis: 2 elektron 2s dan 2 elektron 2p

Total orbital basis = 8

A B

Matriks 8x8 yang dapat dijadikan blok 2x2

$$H = \begin{pmatrix} H_{AA} & H_{AB} \\ H_{BA} & H_{BB} \end{pmatrix}$$

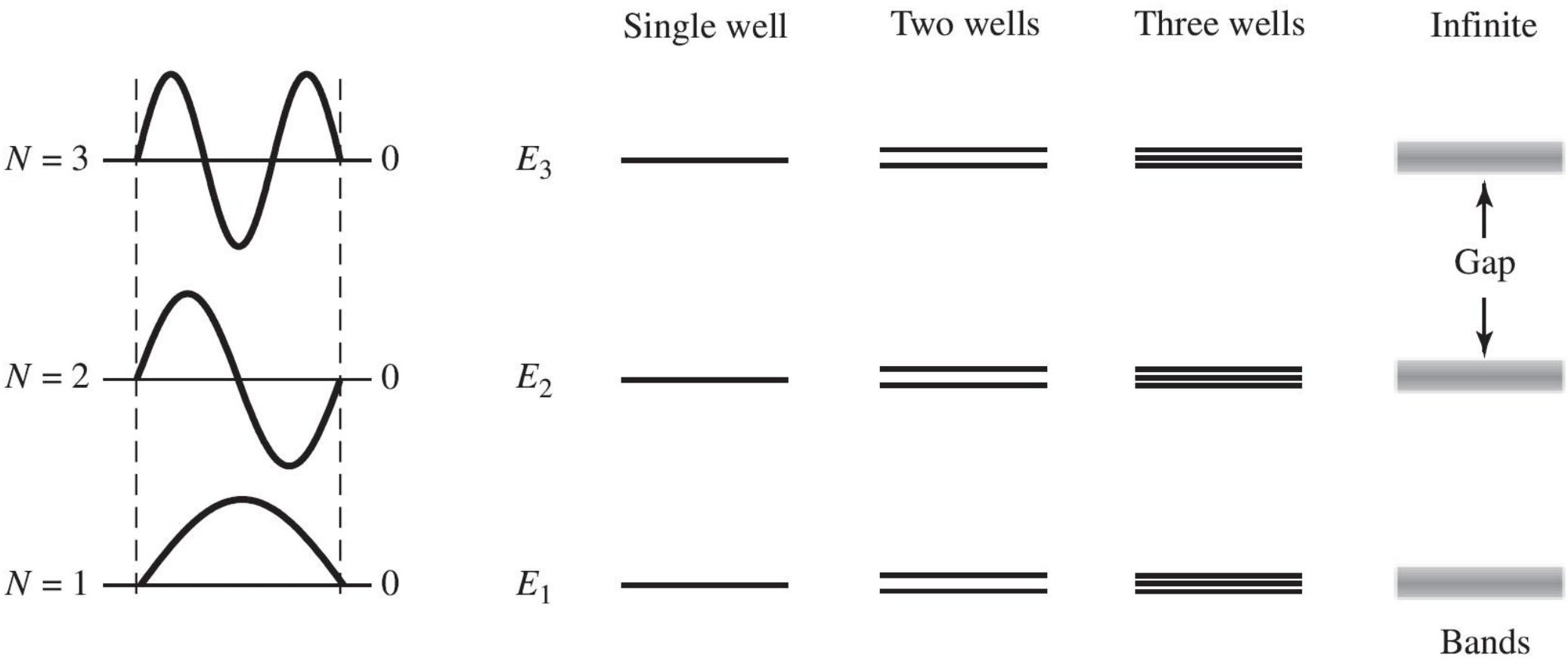
$$H_{AA} = H_{BB} = \begin{array}{c} \begin{array}{cccc} s & p_x & p_y & p_z \end{array} \\ \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \varepsilon & 0 & 0 \\ 0 & 0 & \varepsilon & 0 \\ 0 & 0 & 0 & \varepsilon \end{pmatrix} \end{array} \begin{array}{c} s \\ p_x \\ p_y \\ p_z \end{array}$$

$$H_{AB} = {}^tH_{BA} = \begin{array}{c} \begin{array}{cccc} s & p_x & p_y & p_z \end{array} \\ \begin{pmatrix} t_{2s} & t_{sp} & 0 & 0 \\ -t_{sp} & -t_{pp\sigma} & 0 & 0 \\ 0 & 0 & t_{pp\pi} & 0 \\ 0 & 0 & 0 & t_{pp\pi} \end{pmatrix} \end{array} \begin{array}{c} s \\ p_x \\ p_y \\ p_z \end{array}$$

$$H = \begin{pmatrix} 0 & 0 & 0 & 0 & t_{2s} & t_{sp} & 0 & 0 \\ 0 & \varepsilon & 0 & 0 & -t_{sp} & -t_{pp\sigma} & 0 & 0 \\ 0 & 0 & \varepsilon & 0 & 0 & 0 & t_{pp\pi} & 0 \\ 0 & 0 & 0 & \varepsilon & 0 & 0 & 0 & t_{pp\pi} \\ t_{2s} & -t_{sp} & 0 & 0 & 0 & 0 & 0 & 0 \\ t_{sp} & -t_{pp\sigma} & 0 & 0 & 0 & \varepsilon & 0 & 0 \\ 0 & 0 & t_{pp\pi} & 0 & 0 & 0 & \varepsilon & 0 \\ 0 & 0 & 0 & t_{pp\pi} & 0 & 0 & 0 & \varepsilon \end{pmatrix}$$

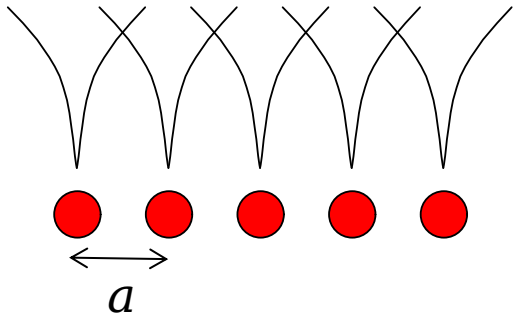
Komponen diagonal: $E_{2p} - E_{2s} \equiv \varepsilon$

Dari Atom/Molekul ke Kristal



Kristal: Sistem periodik atom

$$\left[\frac{-\hbar^2\nabla^2}{2m} + V(r)\right]\psi(r) = E\ \psi(r)$$



$$V(x+a) = V(x)$$

Fungsi periodik

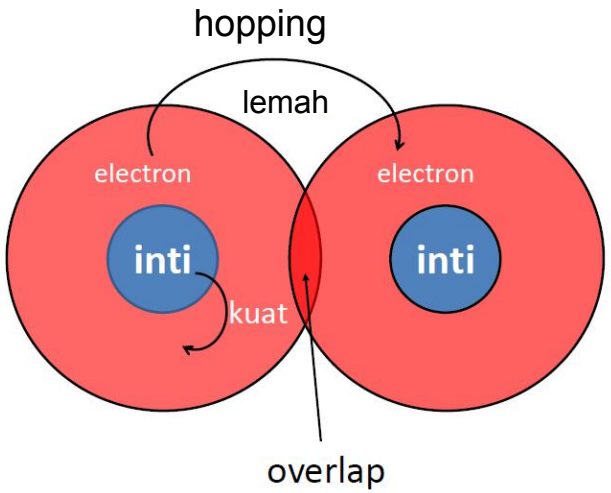
$\lambda = a$

- Aproksimasi tight binding

fungsi gelombang: phase factor × orbital atom

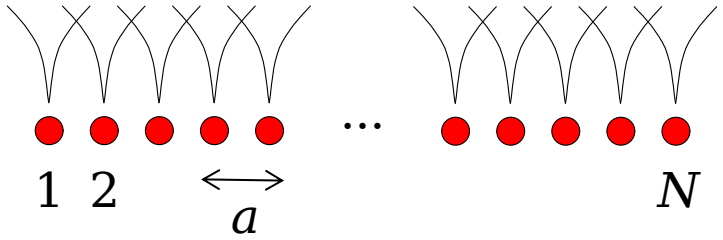
$$\psi(x) = \frac{1}{\sqrt{N}}\sum_{n=1}^{N} e^{ikna}\phi(x-na)$$

$\phi(x-na)$ Orbital atom dengan posisi inti di *x=na*



Fokus pada sebuah *unit cell*, maka kita tidak perlu repot memecahkan masalah ini untuk *N* banyaknya sel
Permasalahan akan tereduksi ke matriks berhingga seperti kasus kombinasi orbital atom untuk molekul

Konsekuensi periodisitas



$$\psi(x+a) = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{ikna} \varphi(x+a-na)$$

$$= e^{ika} \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{ik(n-1)a} \varphi(x+(n-1)a)$$

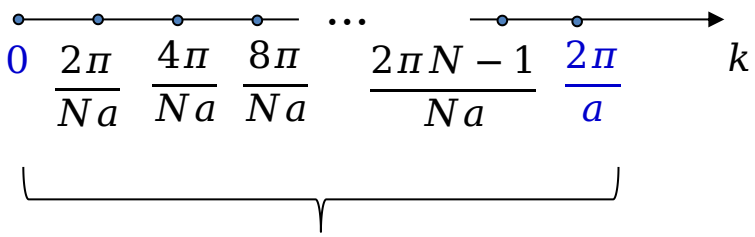
$$= e^{ika} \psi(x)$$

$$\therefore \psi(x+Na) = \psi(x) \Leftrightarrow e^{ikNa} = 1$$

Teorema Bloch

$$H(x+a) = H(x) \quad \Rightarrow \quad \Psi(x+a) = e^{ika}\Psi(x)$$

$$\therefore k = \frac{2\pi m}{Na} (m = 0, \ldots, N-1)$$



Brillouin Zone: memuat kumpulan nilai $\mathbf{k}$

Vektor kisi resiprok 1D: $\mathbf{b} = \frac{2\pi}{a} \hat{\mathbf{a}}$

Kuis

Manakah pernyataan berikut ini yang benar?

(A) Basis pada metode *tight-binding* untuk kristal dapat disusun dari kombinasi linear orbital atom untuk *N* sel satuan disertai faktor fase yang menyatakan fungsi gelombang yang periodik

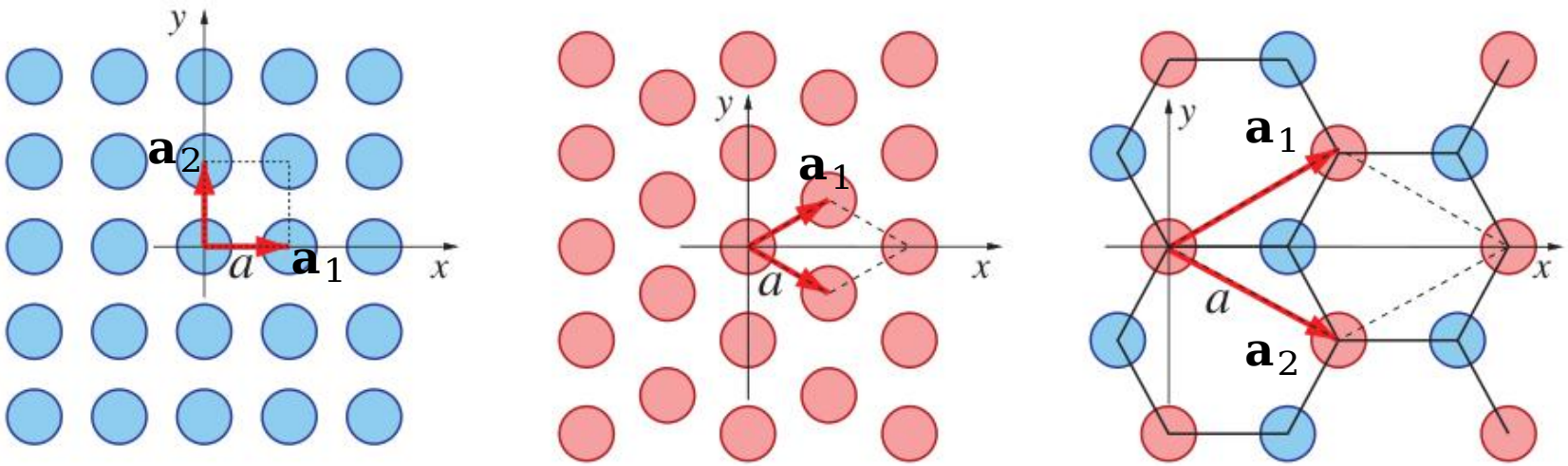
(B) Tak hingga banyaknya sumur potensial dapat membentuk celah energi antara pita-pita energi

(C) Ukuran matriks Hamiltonian yang harus dipecahkan untuk sistem periodik (kristal) dapat tereduksi secara signifikan akibat peninjauan sel satuan sebagai representasi kristal keseluruhan

(D) Semua pernyataan di atas benar

Sel satuan riil dan resiprok

- Sel satuan (*unit cell*): bagian perulangan terkecil dalam kristal



- Vektor satuan $\mathbf{a}_i$ di dalam *unit cell* memiliki pasangan vektor resiprok $\mathbf{b}_j$ di dalam *Brillouin zone*

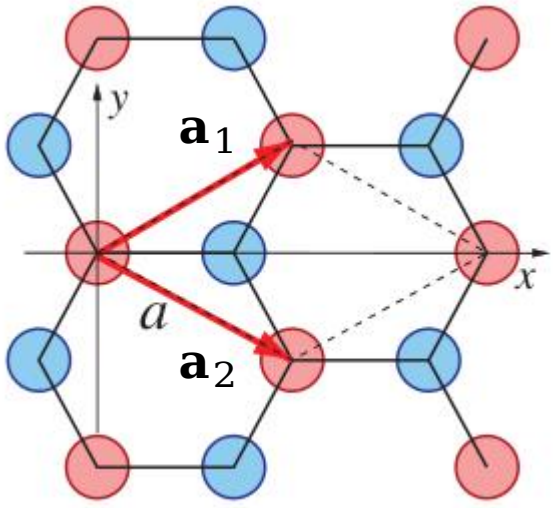
$$\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}$$

Contoh: $\mathbf{a}_1 = a\hat{\mathbf{x}}$ dan $\mathbf{a}_2 = c\hat{\mathbf{y}}$ maka $\mathbf{b}_1 = \frac{2\pi}{a}\hat{\mathbf{x}}$ dan $\mathbf{b}_2 = \frac{2\pi}{c}\hat{\mathbf{y}}$

Kuis

- Diketahui:

$$\mathbf{a}_1 = (\frac{\sqrt{3}}{2}, \frac{1}{2})a, \mathbf{a}_2 = (\frac{\sqrt{3}}{2}, -\frac{1}{2})a$$



Manakah yang merupakan vektor-vektor kisi resiprok dari graphene?

(A) $\mathbf{b}_1 = \left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)\frac{4\pi}{\sqrt{3}a}$ $\mathbf{b}_2 = \left(\frac{1}{2}, -\frac{\sqrt{3}}{2}\right)\frac{4\pi}{\sqrt{3}a}$

(B) $\mathbf{b}_1 = \left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)\frac{4\pi}{\sqrt{3}a}$ $\mathbf{b}_2 = \left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)\frac{4\pi}{\sqrt{3}a}$

(C) $\mathbf{b}_1 = \left(\frac{1}{2}, -\frac{\sqrt{3}}{2}\right)\frac{4\pi}{\sqrt{3}a}$ $\mathbf{b}_2 = \left(\frac{1}{2}, -\frac{\sqrt{3}}{2}\right)\frac{4\pi}{\sqrt{3}a}$

(D) $\mathbf{b}_1 = \left(\frac{1}{2}, -\frac{\sqrt{3}}{2}\right)\frac{4\pi}{\sqrt{3}a}$ $\mathbf{b}_2 = \left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)\frac{4\pi}{\sqrt{3}a}$

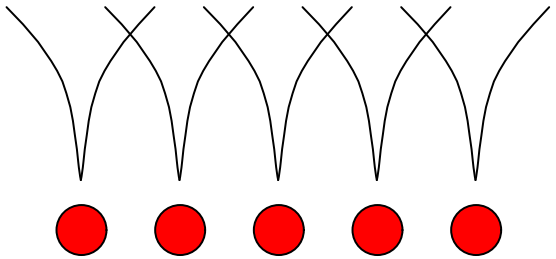
Penerapan TB: Metal 1D

$$\Psi_k(x) = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{ikna} \varphi(x - na)$$

$$E_k = \frac{\langle \Psi_k(x) | H | \Psi_k(x) \rangle}{\langle \Psi_k(x) | \Psi_k(x) \rangle}$$

$$H = -\frac{\hbar^2}{2m} \Delta + V(r)$$

$$V(x+a) = V(x)$$



$$E_k = \frac{\langle \Psi_k(x) | H | \Psi_k(x) \rangle}{\langle \Psi_k(x) | \Psi_k(x) \rangle}$$ nilai harap energi

$$= \frac{\frac{1}{N} \sum_{n,m=1}^{N} e^{ik(n-m)a} \int \varphi^*(x - ma) H \varphi(x - na) dx}{\frac{1}{N} \sum_{n,m=1}^{N} e^{ik(n-m)a} \int \varphi^*(x - ma) \varphi(x - na) dx}$$

$$= \frac{\sum_{n,m=1}^{N} e^{ik(n-m)a} H_{n-m}}{\sum_{n,m=1}^{N} e^{ik(n-m)a} S_{n-m}}$$

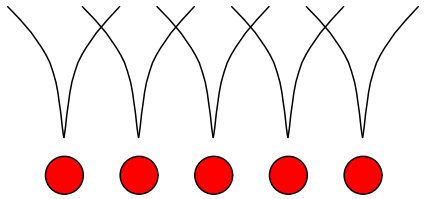
H : *hamiltonian matrix* *S* : *overlap matrix*

$$H_{nm} = H_{n-m,0} \equiv H_{n-m} = \int \varphi^*(x - ma) H \varphi(x - na) dx$$

$$S_{nm} = S_{n-m,0} \equiv S_{n-m} = \int \varphi^*(x - ma) \varphi(x - na) dx$$

Penerapan TB: Metal 1D

- Tinjauan tetangga terdekat



$$E_k = \frac{\sum_{n,m=1}^{N} e^{ik(n-m)a} H_{n-m}}{\sum_{n,m=1}^{N} e^{ik(n-m)a} S_{n-m}}$$

$$= \frac{H_0 + e^{ika} H_1 + e^{-ika} H_1}{S_0}$$

$$= \varepsilon - 2t\cos ka$$

$$(-\pi \le ka \le \pi)$$

pembilang $n = m, m \pm 1 \Rightarrow H_0, H_1$

penyebut $n = m \Rightarrow S_0$

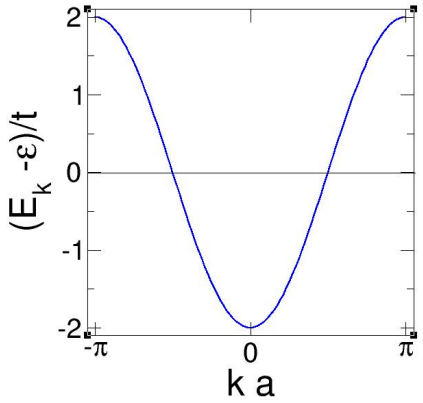
dengan

$$\varepsilon = \frac{H_0}{S_0}, -t = \frac{H_1}{S_0}$$

$$-t < 0$$

$$k = \frac{2\pi m}{Na}$$

$$(m = 0, \ldots, N-1)$$

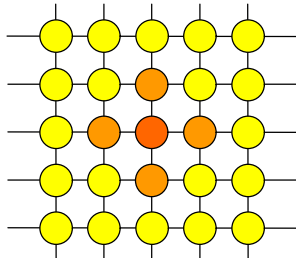


$E(k)$: energy dispersion
$|4t|$: energy band width

Kali ini kita definisikan t positif, tetapi secara keseluruhan *hopping parameter* adalah negatif

Dimensi lebih tinggi?

- 1 atom per unit cell dan 1 orbital
  - vektor perpindahan ke tetangga terdekat $\Delta\mathbf{R}_j = \mathbf{R}_j - \mathbf{R}_0$
  - parameter transfer $\varepsilon = 0, -t = \frac{H_1}{S_0}$
  - hubungan dispersi $E(k) = -t\sum_j e^{-i\mathbf{k}\cdot\mathbf{R}_j}$

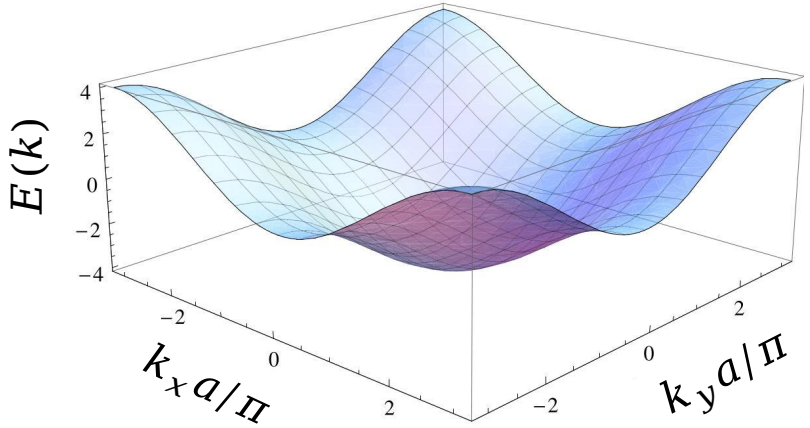


- Contoh kisi persegi 2D

$$\Delta\mathbf{R}_j = (\pm a, 0), (0, \pm a)$$

$$E(k) = -t\left(e^{ik_x a} + e^{-ik_x a} + e^{ik_y a} + e^{-ik_y a}\right)$$

$$= -2t(\cos k_x a + \cos k_y a)$$



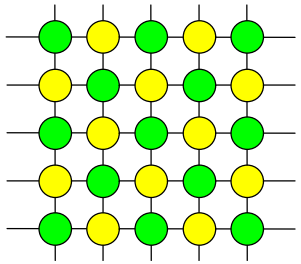
Sejumlah atom dalam 1 sel

- *m* buah atom dalam unit cell→ *m* fungsi Bloch $\Phi_i^k \quad (i = 1, \ldots, m)$

$$\Psi_k = \sum_i C_i \Phi_i^k$$

C_i :variational parameter

$$\Phi_i^k = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}_i} e^{i\mathbf{k}\cdot\Delta\mathbf{R}_i} \varphi_i(\mathbf{r} - \mathbf{R}_i)$$



$$E_k = \frac{\langle \Psi_k | H | \Psi_k \rangle}{\langle \Psi_k | \Psi_k \rangle} = \frac{\sum_{i,j} C_i^* C_j H_{ij}}{\sum_{i,j} C_i^* C_j S_{ij}}$$

$$S_{ij} = \langle \Phi_i^k | \Phi_i^k \rangle \mathbf{S}$$:*overlap matrix*

$$H_{ij} = \langle \Phi_i^k | H | \Phi_j^k \rangle \mathbf{H}$$:*Hamiltonian matrix*

C secara umum kompleks sehingga perlu pisahkan turunan *C* dan *C**

Prinsip variasi

$$\frac{\partial E_k}{\partial C_i^*} = \frac{\sum_j C_j H_{ij}}{\sum_{i,j} C_i^* C_j S_{ij}} - \frac{\sum_{i,j} C_i^* C_j H_{ij}}{\left(\sum_{i,j} C_i^* C_j S_{ij}\right)^2} \times \sum_j C_j S_{ij} = 0, (i = 1, \cdots, N)$$

$$\frac{\partial E_k}{\partial C_i^*} = 0, (i = 1, \cdots, N)$$

Secular equation

Kondisi variasional → *m* buah pers. simultan $\Psi_k = \sum_i C_i \Phi_i^k, \quad \rightarrow \quad E_k = \dfrac{\sum_{i,j} C_i^* C_j H_{ij}}{\sum_{i,j} C_i^* C_j S_{ij}}$

Prinsip variasi

$$\frac{\partial E_k}{\partial C_i^*} = \frac{\sum_j C_j H_{ij}}{\sum_{i,j} C_i^* C_j S_{ij}} - \frac{\sum_{i,j} C_i^* C_j H_{ij}}{\left(\sum_{i,j} C_i^* C_j S_{ij}\right)^2} \times \sum_j C_j S_{ij} = 0, \quad (i = 1, \ldots, m)$$

$$E_k = \frac{\sum_{i,j} C_i^* C_j H_{ij}}{\sum_{i,j} C_i^* C_j S_{ij}}$$

$$\sum_j C_j H_{ij} - E_k \sum_j C_j S_{ij} = 0, \quad (i = 1, \ldots, m)$$

$$(\mathbf{H} - E_k \mathbf{S})\mathbf{C} = 0$$

Overlap matrix $\mathbf{S} = \{S_{ij}\}, \ \mathbf{C} = {}^{\mathrm{t}}\{C_j\}$

Hamiltonian matrix $\mathbf{H} = \{H_{ij}\}$

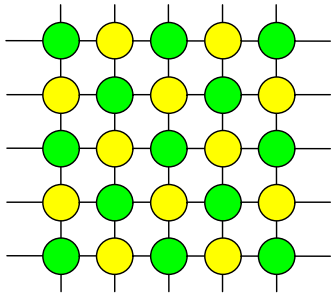
$$\mathbf{C} \neq 0 \Leftrightarrow \det(\mathbf{H} - E_k \mathbf{S}) = 0$$

secular equation

Esensi metode *tight-binding*:
Peroleh H dan S pada tiap *k*
dan pecahkan pers. sekuler

Contoh pada kisi persegi

Dua atom, A and B, dalam kisi persegi



overlap matrix $\mathbf{S} = \delta_{ij}$, *(unit matrix)*

Hamiltonian matrix $\mathbf{H} = \{H_{ij}\}$

$$H_{AA} = +\Delta/2,\ H_{BB} = -\Delta/2$$

$$H_{AB} = -t\left(e^{ik_x a} + e^{-ik_x a} + e^{ik_y a} + e^{-ik_y a}\right)$$

$$H_{BA} = H_{AB}^{*}$$

$$\Psi_k = \sum_i C_i \Phi_i^k,\ (i = A, B)$$

$$\det(\mathbf{H} - E_k\mathbf{S}) = \begin{vmatrix} +\Delta/2 - E_k & H_{AB} \\ H_{BA} & -\Delta/2 - E_k \end{vmatrix}$$

$$= E_k^2 - (\Delta/2)^2 - |H_{AB}|^2$$

$$= 0$$

$$\therefore E_k = \pm\sqrt{(\Delta/2)^2 + |H_{AB}|^2}$$

$$|H_{AB}|^2 = 4t^2(\cos k_x a + \cos k_y a)^2$$

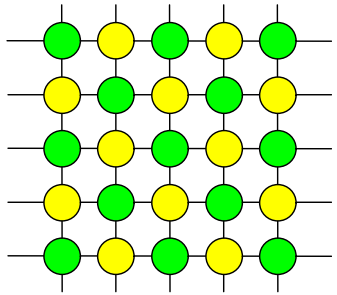
$$-\frac{\pi}{2a} \le k_x, k_y \le \frac{\pi}{2a}$$ (sel satuan berbatas *2a*)

Kuis

- Diketahui: $E_k = \pm\sqrt{(\Delta/2)^2 + |H_{AB}|^2}$

$$|H_{AB}|^2 = 4t^2(\cos k_x a + \cos k_y a)^2$$

$$-\frac{\pi}{2a} \le k_x, k_y \le \frac{\pi}{2a}$$



Berapakah nilai celah energi (*band gap*) dari sistem tersebut?

(A) $|\Delta|/2$ (B) $|\Delta|$

(C) $2|\Delta|$ (D) $4|\Delta|$