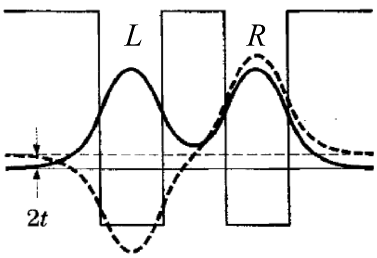
TIGHT-BINDING MODEL

Two Wells: Diatomic Molecule



$$E_- = \varepsilon - \frac{c}{1+s} - \frac{t}{1+s}$$

$$E_+ = \varepsilon - \frac{c}{1-s} + \frac{t}{1-s}$$

- Energy gap: $E_+ - E_- = \frac{c}{1+s} - \frac{c}{1-s} + \frac{t}{1-s} + \frac{t}{1+s} \approx 2t$
- Oscillation frequency: $\omega = \frac{|E_+ - E_-|}{\hbar} = \frac{2|t|}{\hbar}$

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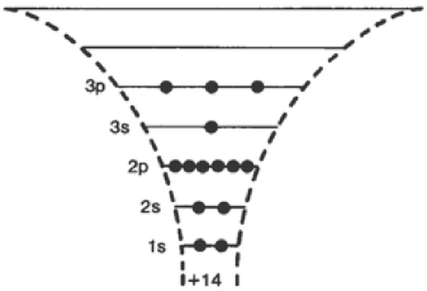
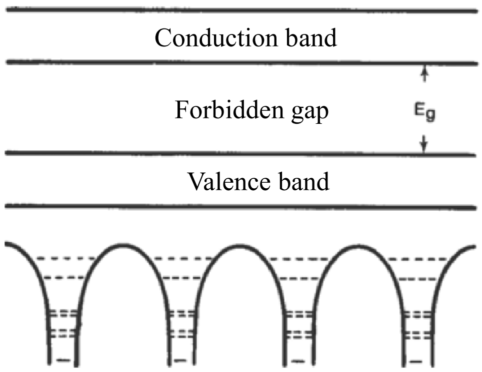
Silicon Atom and 1-D Lattice

- As the spacing of the silicon atoms reduces to a few angstroms, the discrete energy levels broaden into energy bands.



Isolated silicon atom



1-D silicon lattice

Row of Wells / Atoms

- Hamiltonian:

$$\hat{H} = \hat{T} + \sum_n \hat{V}_n$$

$\hat{T}$: Kinetic energy operator

$\hat{V}_n$: Potential energy operator of well n

- The orbital associated with well n obeys:

$$\left(\hat{T} + \hat{V}_n\right)\phi_n = \varepsilon\phi_n$$

New Wavefunctions

- Neglecting contributions from other orbitals:

$$\psi = \sum_n a_n \phi_n$$

- Using Bloch's theorem:

$$\psi_k = \sum_n a_n^k \phi_n, \quad a_n^k = e^{ikx} = e^{ikna}$$

Schrodinger's Equation

$$\hat{H}\sum_n a_n^k \phi_n = E(k)\sum_n a_n^k \phi_n$$

$$\hat{H}\sum_n e^{ikna} \phi_n = E(k)\sum_n e^{ikna} \phi_n$$

- Multiply both sides by ϕ_m* and integrate:

$$\sum_n H_{mn} e^{ikna} = E(k)\sum_n S_{mn} e^{ikna}$$

$$H_{mn} = \int \phi_m^* \hat{H} \phi_n, \quad S_{mn} = \int \phi_m^* \phi_n$$

Ha = ESa

Matrix Elements

$$H_{mn} = \int \phi_m^* \left(\hat{T} + \hat{V}_n + \sum_{l,l\neq n} \hat{V}_l \right) \phi_n dx = \varepsilon S_{mn} + \sum_{l,l\neq n} V_{mn}^l$$

- The interactions of the far atoms can be neglected. We assume that only the nearest neighbors are important.

- Diagonal elements: $H_{mm} = \varepsilon S_{mm} + V_{mm}^{m-1} + V_{mm}^{m+1} = \varepsilon - 2c$

$$S_{mm} = \int \phi_m^* \phi_m = 1 \qquad V_{mm}^{m-1} = \int \phi_m^* \hat{V}_{m-1} \phi_m = -c$$

$$V_{mm}^{m+1} = \int \phi_m^* \hat{V}_{m+1} \phi_m = -c$$

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Matrix Elements

- Off-diagonal elements:

$$H_{m,m+1} = \varepsilon S_{m,m+1} + V_{m,m+1}^m = \varepsilon s - t = H_{m,m-1}$$

$$S_{m,m+1} = \int \phi_m^* \phi_{m+1} = s = S_{m,m-1}$$

$$V_{m,m+1}^m = \int \phi_m^* \hat{V}_m \phi_{m+1} = -t = V_{m,m-1}^m$$

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Solution

- Schrodinger equation:

$$\sum_n H_{mn} e^{ikna} = E(k) \sum_n S_{mn} e^{ikna}$$

- Left-hand side:

$$\sum_n H_{mn} e^{ikna} \approx H_{mm} e^{ikma} + H_{m,m+1} e^{ik(m+1)a} + H_{m,m-1} e^{ik(m-1)a}$$

$$= \left(H_{mm} + H_{m,m+1} e^{ika} + H_{m,m-1} e^{-ika} \right) e^{ikma}$$

$$= \left[\varepsilon - 2c + (\varepsilon s - t) e^{ika} + (\varepsilon s - t) e^{-ika} \right] e^{ikma}$$

$$= \left[\varepsilon - 2c + 2(\varepsilon s - t) \cos ka \right] e^{ikma}$$

Solution

- Right-hand side:

$$\sum_n S_{mn} e^{ikna} \approx S_{mm} e^{ikma} + S_{m,m+1} e^{ik(m+1)a} + S_{m,m-1} e^{ik(m-1)a}$$

$$= e^{ikma} + s e^{ik(m+1)a} + s e^{ik(m-1)a}$$

$$= \left(1 + s e^{ika} + s e^{-ika} \right) e^{ikma} = \left(1 + 2s \cos ka \right) e^{ikma}$$

- Energy level:

$$E(k) = \frac{\sum_n H_{mn} e^{ikna}}{\sum_n S_{mn} e^{ikna}} = \frac{\varepsilon - 2c + 2(\varepsilon s - t) \cos ka}{1 + 2s \cos ka}$$

$$= \varepsilon - 2 \frac{c + t \cos ka}{1 + 2s \cos ka} \approx \varepsilon - 2t \cos ka$$

Energy

- One dimension: $E_k = \varepsilon - t\left(e^{ik_x a} + e^{-ik_x a}\right)$
  $= \varepsilon - 2t\cos k_x a$

- Two dimensions: $E_k = \varepsilon - t\left(e^{ik_x a} + e^{-ik_x a} + e^{ik_y a} + e^{-ik_y a}\right)$
  $= \varepsilon - 2t\left(\cos k_x a + \cos k_y a\right)$

- Three dimensions:

$$E_k = \varepsilon - t\left(e^{ik_x a} + e^{-ik_x a} + e^{ik_y a} + e^{-ik_y a} + e^{ik_z a} + e^{-ik_z a}\right)$$
$$= \varepsilon - 2t\left(\cos k_x a + \cos k_y a + \cos k_z a\right)$$

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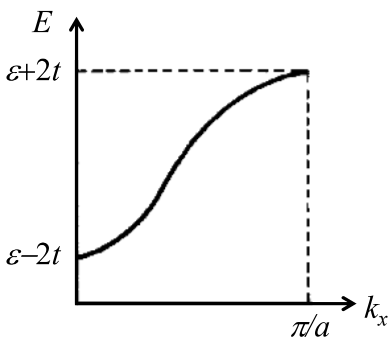
E-k Relation

- One dimension:



- Near the bottom:

$$\cos k_x a \approx 1 - \frac{k_x^2 a^2}{2}$$

$$E_k = \varepsilon - 2t\cos k_x a$$
$$= \varepsilon - 2t\left(1 - \frac{k_x^2 a^2}{2}\right)$$
$$= \varepsilon - 2t + t k_x^2 a^2$$

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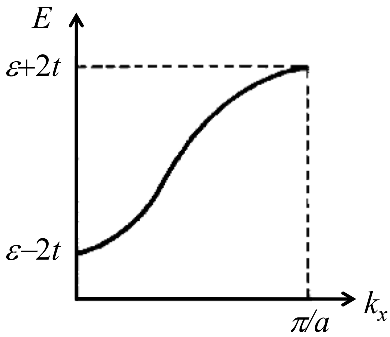
E-k Relation

- One dimension:



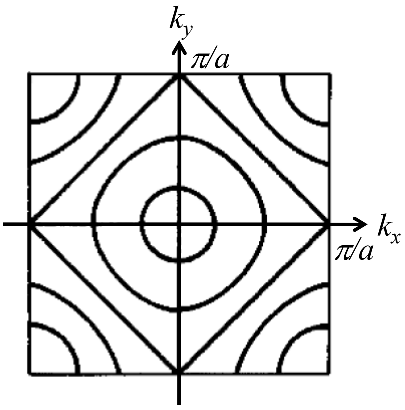
- Near the top:

$$k_x = \frac{\pi}{a} - k_x'$$

$$\begin{aligned} E_k &= \varepsilon - 2t\cos k_x a \\ &= \varepsilon - 2t\cos\left[\left(\frac{\pi}{a} - k_x'\right)a\right] \\ &= \varepsilon + 2t\cos k_x' a \\ &= \varepsilon + 2t - t k_x'^2 a^2 \end{aligned}$$

E-k Relation

- Two dimensions:



- Near the bottom:

$$\cos k_x a \approx 1 - \frac{k_x^2 a^2}{2}$$

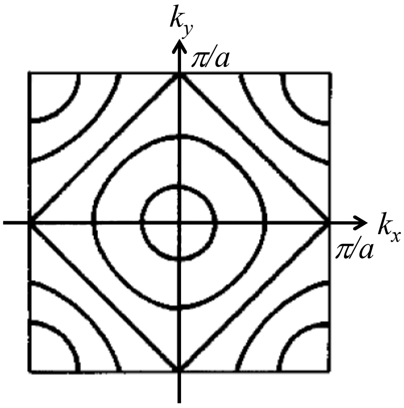
$$\cos k_y a \approx 1 - \frac{k_y^2 a^2}{2}$$

$$\begin{aligned} E_k &= \varepsilon - 2t\left(\cos k_x a + \cos k_y a\right) \\ &= \varepsilon - 2t\left(1 - \frac{k_x^2 a^2}{2} + 1 - \frac{k_y^2 a^2}{2}\right) \\ &= \varepsilon - 4t + t\left(k_x^2 + k_y^2\right)a^2 \end{aligned}$$

$$k_x^2 + k_y^2 = \frac{E_k - \varepsilon + 4t}{ta^2}$$

E-k Relation

- Two dimensions:



- Near the top:

$$k_x = \frac{\pi}{a} - k'_x$$

$$k_y = \frac{\pi}{a} - k'_y$$

$$\begin{aligned} E_k &= \varepsilon + 2t\left(\cos k'_x a + \cos k'_y a\right) \\ &= \varepsilon + 2t\left(1 - \frac{k'^2_x a^2}{2} + 1 - \frac{k'^2_y a^2}{2}\right) \\ &= \varepsilon + 4t - t\left(k'^2_x + k'^2_y\right)a^2 \end{aligned}$$

$$k'^2_x + k'^2_y = \frac{\varepsilon + 4t - E_k}{ta^2}$$