Quantum wire, 2D confinement, 1D electronic system

\[ \psi = A \sin k_x x \cdot \sin k_y y \cdot e^{ik_z z} \]
\[ E = \frac{\hbar^2}{8m_e} \left( \frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} \right) + \frac{\hbar^2}{2m_e} k_z^2 \]
\[ D(E) = \sqrt{2m_e^*} \frac{E^{-1/2}}{\pi \hbar L_x L_y} \]
\[ k_y = \frac{\pi m_{1d}}{2} \]

\[ E_{g,\text{wire}} = E_{g,0} + \frac{\hbar^2}{8} \left( \frac{1}{m_e} + \frac{1}{m_h} \right) \left( \frac{1}{L_x^2} + \frac{1}{L_y^2} \right) \]
Quantum wire, 2D confinement, 1D electronic system

\[ V_{1D} = \frac{2\pi}{L} \]

Density of states per unit length:

\[
\frac{2dk}{2\pi L} \frac{1}{L_x L_y} \times 2 = \frac{2dk}{\pi L_x L_y} \\
= \frac{2}{\pi L_x L_y} \left( \frac{2mE}{\hbar^2} \right)^{-1/2} \frac{m}{\hbar^2} dE \\
= \frac{\sqrt{2m^*}}{\pi \hbar L_x L_y} E^{-1/2} dE
\]

Quantum Confinement and Dimensionality
Quantum dot, 3D confinement, 0D electronic system

\[ \psi = A \sin(k_x x) \sin(k_y y) \sin(k_z z) \]

\[ E = \frac{\hbar^2}{8m_e} \left( \frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2} \right) \]

Discrete states

Quantum Confinement and Dimensionality
Quantum dots

Discrete atomic-like density of states

CdS quantum dots versus dot size $d$ at 4.2K

Examples:
1. Semiconductor doped glass (Colour glass filters & stained glass)
2. Self-organized III-V quantum dots (eg InAs/GaAs)
\[ E_{g,\text{well}} = E_{g,\text{o}} + \frac{\hbar^2}{8L_z^2} \left( \frac{1}{m_c} \frac{1}{m_h^*} \right) \]

\[ E_{g,\text{wire}} = E_{g,\text{o}} + \frac{\hbar^2}{8} \left( \frac{1}{m_c^*} \frac{1}{m_h^*} \right) \frac{L_z^2}{L_y^2} \]

\[ \Delta E_g \]
\[\psi = A \sin k_z z \cdot e^{i(k_x x + k_y y)}\]

\[E = \frac{\hbar^2 n_z^2}{8m_e L_z^2} + \frac{\hbar^2}{2m_e} (k_x^2 + k_y^2)\]

\[\psi = A \sin k_x x \cdot \sin k_y y \cdot e^{i k_z z}\]

\[E = \frac{\hbar^2}{8m_e} \left( \frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} \right) + \frac{\hbar^2}{2m_e} k_z^2\]

\[\psi = A \sin k_x x \cdot \sin k_y y \cdot \sin k_z z\]

\[E = \frac{\hbar^2}{8m_e} \left( \frac{n_x^2}{L_x} + \frac{n_y^2}{L_y} + \frac{n_z^2}{L_z} \right)\]
<table>
<thead>
<tr>
<th>State</th>
<th>2D $E/E_0$</th>
<th>1D $E/E_0$</th>
<th>Degenerate States</th>
<th>0D $E/E_0$</th>
<th>Degenerate States</th>
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<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>2</td>
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<td>1</td>
<td>8</td>
<td>1</td>
<td>(2,2,1)</td>
</tr>
<tr>
<td>4</td>
<td>16</td>
<td>1</td>
<td>10</td>
<td>2</td>
<td>(3,1,1)</td>
</tr>
<tr>
<td>5</td>
<td>25</td>
<td>1</td>
<td>13</td>
<td>2</td>
<td>(3,2,2)</td>
</tr>
<tr>
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<td>(4,1,1)</td>
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<tr>
<td>7</td>
<td>49</td>
<td>1</td>
<td>18</td>
<td>1</td>
<td>(3,3,3)</td>
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<tr>
<td>8</td>
<td>64</td>
<td>1</td>
<td>20</td>
<td>2</td>
<td>(4,2,1)</td>
</tr>
<tr>
<td>9</td>
<td>81</td>
<td>1</td>
<td>25</td>
<td>2</td>
<td>(4,3,1)</td>
</tr>
<tr>
<td>10</td>
<td>100</td>
<td>1</td>
<td>26</td>
<td>2</td>
<td>(5,1,1)</td>
</tr>
</tbody>
</table>

**Tight Binding Model**

Calculation of Energy Band

Reading: **Burdett Chpt 1-3**  
**Hoffman p1-21**

For MO Theory:  
**Chemical structure and bonding (Gray/Decock)**
Molecular Orbital Theory

Antibonding Orbital, $\sigma^*$

Bonding Orbital, $\sigma$

H$_2$ molecular orbitals

H atomic orbitals

Energy
Chem 253, UC, Berkeley

Diatomic Molecules

Chem 253, UC, Berkeley

Orbital Interactions: Key Points

- The overlap of two atomic orbitals is dependent upon:
  - symmetry of the orbitals
  - distance between the orbitals
  - spatial extent of the orbitals
  - the energy difference between orbitals

- Increasing the overlap (spatial and energetic) leads to the following:
  - Stabilization of the bonding MO
  - Destabilization of the antibonding MO
  - The antibonding MO is destabilized to a greater extent than the bonding MO is stabilized

- The spatial overlap in a bond depends upon symmetry
  - It decreases as the number of nodal planes increases, $\sigma > \pi > \delta$
  - $\pi$ and particularly $\delta$ bonds are more sensitive to changes in bond angle
**Elementary Band Theory for Molecules**

**Schrödinger equation**

\[ \hat{H}\psi = E\psi \]

Solving the Schrödinger equation after applying simplifications

**LCAO**: linear combination of atomic wavefunctions, the Atomic Orbitals \( \phi \)

\[ \psi = \sum c_i \phi_i \]

\( \phi \) is normalized, thus \( \int \phi_i^2 d\tau = 1 \)

with \( d\tau = dx dy dz \)

Calculate the expectation value of \( \hat{H} \):

\[ E = \frac{\int \psi \hat{H}\psi d\tau}{\int \psi^2 d\tau} \]

For a minimal \( E \): \( \frac{\partial E}{\partial c_i} = 0 \)

**Case studies**: 1) the diatomic case

\[ \psi = \sum \psi_i = c_1 \phi_1 + c_2 \phi_2 \]

For a minimal \( E \): \( \frac{\partial E}{\partial c_1} = 0 \), i.e.

\( \frac{\partial E}{\partial c_1} = 0 \) and \( \frac{\partial E}{\partial c_2} = 0 \)

=> two solutions

\[ E = \frac{\int \psi \hat{H}\psi d\tau}{\int \psi^2 d\tau} \]

\[ \int \psi \hat{H}\psi d\tau = \int (c_1 \phi_1 + c_2 \phi_2)\hat{H}(c_1 \phi_1 + c_2 \phi_2) d\tau \]

Using the analogy \( (a + b)^2 = a^2 + 2ab + b^2 \):

\[ = \int (c_1^2 \phi_1^2 \hat{H}\phi_1 + 2c_1c_2 \phi_1 \phi_2 \hat{H}\phi_2 + c_2^2 \phi_2^2 \hat{H}\phi_2) d\tau \]

\[ = c_1^2 \int \phi_1^2 \hat{H}\phi_1 d\tau + 2c_1c_2 \int \phi_1 \phi_2 \hat{H}\phi_2 d\tau + c_2^2 \int \phi_2^2 \hat{H}\phi_2 d\tau \]

Coulomb-integral \( \alpha_1 < 0 \)

Coulomb-integral \( \alpha_2 < 0 \)

resonance-integral \( \beta_{12} < 0 \) if bonding
Case studies: the diatomic case, continued

\[ \psi = \sum_i c_i \phi_i = c_1 \phi_1 + c_2 \phi_2 \]

Numerator (I):

\[ \int \psi \hat{H} \psi \text{d}t = c_1^2 \alpha_1 + 2c_1c_2 \beta_{12} + c_2^2 \alpha_2 \]

Denominator (II):

\[ \int \psi^2 \text{d}t = \int (c_1 \phi_1 + c_2 \phi_2)^2 \text{d}t \]

\[ = \int (c_1^2 \phi_1^2 + 2c_1c_2 \phi_1 \phi_2 + c_2^2 \phi_2^2) \text{d}t \]

\[ = c_1^2 \int \phi_1^2 \text{d}t + 2c_1c_2 \int \phi_1 \phi_2 \text{d}t + c_2^2 \int \phi_2^2 \text{d}t \]

\[ = 1 \quad \text{overlap} \quad = 1 \]

\[ S_{12} \geq 0 \quad \text{if bonding} \]

\[ \Rightarrow \int \psi^2 \text{d}t = c_1^2 + 2c_1c_2S_{12} + c_2^2 \]

\[ \frac{\partial E}{\partial c_1} = 0 \]

\[ \frac{\partial E}{\partial c_1} = \frac{\partial}{\partial c_1} \left( \frac{c_1^2 \alpha_1 + 2c_1c_2 \beta_{12} + c_2^2 \alpha_2}{c_1^2 + 2c_1c_2S_{12} + c_2^2} \right) = 0 \]

Case studies: the diatomic case, continued

\[ (\alpha_1 - E)c_1 + (\beta_{12} - ES_{12})c_2 = 0 \]

\[ (\beta_{12} - ES_{12})c_1 + (\alpha_2 - E)c_2 = 0 \]

Secular determinant = 0

\[
0 = \begin{vmatrix}
\alpha_1 - E & \beta_{12} - ES_{12} \\
\beta_{12} - ES_{12} & \alpha_2 - E
\end{vmatrix}
\]

General rule:

\[ 0 = \begin{vmatrix}
A & B \\
C & D
\end{vmatrix} = AD - BC \]

\[ 0 = (\alpha_1 - E)(\alpha_2 - E) - (\beta_{12} - ES_{12})(\beta_{12} - ES_{12}) \]

Case studies: 1a) the diatomic homoatomic case, e.g. H_2

\[ \alpha_1 = \alpha_2 = \alpha \]

\[ 0 = (\alpha - E)(\alpha - E) - (\beta - ES)(\beta - ES) = (\alpha - E)^2 - (\beta - ES)^2 \]

\[ \Rightarrow (\alpha - E) = \pm (\beta - ES) \]
Case studies: the diatomic homoatomic case, e.g. H$_2$

\[ \alpha - E = \pm (\beta - ES): \text{two solutions, A and B} \]

<table>
<thead>
<tr>
<th>A</th>
<th>B</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \alpha - E = -(\beta - ES) )</td>
<td>( \alpha - E = \beta - ES )</td>
</tr>
<tr>
<td>( \alpha + \beta = E(1 + S) )</td>
<td>( \alpha - \beta = E(1 - S) )</td>
</tr>
<tr>
<td>( E = (\alpha + \beta)/(1+S) )</td>
<td>( E = (\alpha - \beta)/(1-S) )</td>
</tr>
<tr>
<td>( c_1 = 1/\sqrt{2(1 + S)} = c_2 )</td>
<td>( c_1 = 1/\sqrt{2(1 - S)} = -c_2 )</td>
</tr>
</tbody>
</table>

Calculated without any approximation

"He$_2"$

Case studies: more complex molecules

Conjugated molecules, e.g. ethene, C$_2$H$_4$, and butadiene, C$_4$H$_6$

\[ \text{C}_2\text{H}_4 \]

VB: sp$^2$ for each C atom

Consider only the \( \pi \) bonds:

\[ \psi = \sum_i c_i \phi_i = c_1 \phi_1 + c_2 \phi_2 \]

Problem solved by analogy:

\[ E_1 = (\alpha + \beta)/(1+S), \ E_2 = (\alpha - \beta)/(1-S) \]

\[ \text{C}_4\text{H}_6 \]

\[ \psi = \sum_i c_i \phi_i = c_1 \phi_1 + c_2 \phi_2 + c_3 \phi_3 + c_4 \phi_4 \]

Secular determinant = 0

\[
0 = \begin{bmatrix}
\alpha_1 - E & \beta_{12} - ES_{12} & \beta_{13} - ES_{13} & \beta_{14} - ES_{14} \\
\beta_{21} - ES_{21} & \alpha_2 - E & \beta_{23} - ES_{23} & \beta_{24} - ES_{24} \\
\beta_{31} - ES_{31} & \beta_{32} - ES_{32} & \alpha_3 - E & \beta_{34} - ES_{34} \\
\beta_{41} - ES_{41} & \beta_{42} - ES_{42} & \beta_{43} - ES_{43} & \alpha_4 - E
\end{bmatrix}
\]
$C_4H_6$, continued ....

Problem 'solution' by approximation(s):
1. approx.: set $\beta_i = 0$ unless adjacent atoms → **Extended Hückel**
2. approx.: set $S_j = 0$ → **Simple Hückel**

Hückel determinant: $| H_i - \alpha_i | = 0$

Extended Hückel determinant: $| H_i - S_j \beta_i | = 0$

$H_{ii} = \alpha_i = \int \phi_i \phi_i^* d\tau$ Coulomb integral = - ionization potential

$H_{ij} = \beta_{ij} = \int \phi_i \phi_j^* d\tau$ resonance integral

$H_{ii}$ is proportional to the average of $H_{ii}$ and $H_{jj}$

Ionization potential [eV] examples for Hückel calculations

<table>
<thead>
<tr>
<th></th>
<th>B</th>
<th>C</th>
<th>N</th>
<th>O</th>
<th>F</th>
</tr>
</thead>
<tbody>
<tr>
<td>2s</td>
<td>14.0</td>
<td>19.4</td>
<td>25.6</td>
<td>32.3</td>
<td>40.2</td>
</tr>
<tr>
<td>2p</td>
<td>8.3</td>
<td>10.6</td>
<td>13.2</td>
<td>15.8</td>
<td>18.6</td>
</tr>
</tbody>
</table>

$C_4H_6$, continued ....

ethene, or H$_2$:

$E_1 = (\alpha + \beta)/(1+S)$, $E_2 = (\alpha - \beta)/(1-S)$ no approx.

$E_1 = (\alpha + \beta)/(1+S)$, $E_2 = (\alpha - \beta)/(1-S)$ Extended Hückel

$E_1 = (\alpha + \beta)$, $E_2 = (\alpha - \beta)$ Simple Hückel

$C_4H_6$, secular determinant in the **Simple Hückel** approximation

\[
0 = \begin{vmatrix}
\alpha - \beta & 0 & 0 \\
\beta & \alpha - \beta & 0 \\
0 & \beta & \alpha - \beta \\
0 & 0 & \beta & \alpha - \beta
\end{vmatrix}
\]
$C_4H_6$, continued ....

$$0 = (\alpha - E)^4 - 3(\alpha - E)\beta^2 + 4\beta^4$$

solve in analogy to

$$ax^4 + bx^2 + c = 0,$$ with $u = x^2$:

$$au^2 + bu + c = 0$$

$$\Rightarrow E = \alpha \pm 1.62\beta, \ E = \alpha \pm 0.62\beta$$

**Simple Hückel**

---

**General scheme for 'linear' polyenes**

**Simple Hückel**

\[ C_2H_4: E = \alpha \pm \beta; \ C_3H_6: E = \alpha \pm \sqrt{2}\beta, \ \alpha; \]

\[ C_4H_6: \alpha \pm 1.6\beta, \ \alpha \pm 0.6\beta; \ C_{6N+2}: E = \alpha \pm 2\beta, \ldots \]
General scheme for 'linear' polyenes

CₙHₙ₋₂: n atoms, n π orbitals, j energy levels with j = 1, 2, 3, ..., n

\[ E_j = \alpha + 2\beta \cos\left(\frac{j\pi}{n+1}\right) \]

Examples:
- ethene, C₂H₄, n = 2:
  \[ E_1 = \alpha + 2\beta \cos\frac{\pi}{3} = \alpha + \beta \]
  \[ E_2 = \alpha + 2\beta \cos\frac{2\pi}{3} = \alpha - \beta \]
- allyl, C₃H₅, n = 3:
  \[ E_1 = \alpha + 2\beta \cos\frac{\pi}{4} = \alpha + \sqrt{2}\beta \quad ... \]

Cyclic (CₙHₙ) vs. 'linear' polyenes (CₙHₙ₋₂)
e.g., cyclobutadiene vs. butadiene
different secular determinants!

Cyclic vs. 'linear' polyenes

\[ \begin{array}{ccc|cc|cc}
\alpha - \xi & \beta & 0 & \beta \\
\beta & \alpha - \xi & \beta & 0 \\
0 & \beta & \alpha - \xi & \beta \\
\beta & 0 & \beta & \alpha - \xi \\
\end{array} \]

\[ \begin{array}{ccc|cc|cc}
\alpha - \xi & \beta & 0 & 0 \\
\beta & \alpha - \xi & \beta & 0 \\
0 & \beta & \alpha - \xi & \beta \\
0 & 0 & \beta & \alpha - \xi \\
\end{array} \]

\[ 0 = E = \alpha \pm 2\beta, \alpha, \alpha \]
=> \[ E = \alpha \pm 1.62\beta, E = \pm 0.62\beta \]

CₙHₙ: n atoms, n π orbitals, j energy levels with
- j = ±1, ±2, ±3, ..., ±n/2 if n even
- j = 0, ±1, ±2, ±3, ..., ±(n-1)/2 if n odd

\[ E_j = \alpha + 2\beta \cos\left(\frac{2j\pi}{n}\right) \]

Cyclobutadiene: n = 4, j = ±1, ±2
\[ => E_2 = \alpha + 2\beta \cos\left(\frac{4\pi}{4}\right) = \alpha - 2\beta \]
Cyclic polyenes

\[ E_j = \alpha + 2\beta \cos \left( \frac{2\pi j}{n} \right) \]

Simple Hückel

**Frost's circles:**

tool for estimating the \( \pi \) MO's for cyclic polyenes

Construction:

1) draw the polyene schematically, with one vertex at the bottom
2) draw a circle around the center, which touches all vertices

=> DONE! The energy levels are, where the corners of the polyene touch the circle.

\[ \text{antibonding orbitals} \]
\[ \text{nonbonding energy level; } E = \alpha \]
\[ \text{bonding orbitals} \]
Chem 253, UC, Berkeley

More molecules

Simple Hückel
Elementary Band Theory for Extended Solids

Energy bands in solids arise from overlapping
atomic orbitals \(\rightarrow\) crystal orbitals (that make up the bands)

Recipe: use LCAO (tight binding) approach

Crystal = regular periodic array \(\rightarrow\) translational symmetry

Periodic boundary condition requires: \(\psi(x+Na) = \psi(x)\).
I.e. each wavefunction must be symmetry equivalent to the one in the neighboring cells.
A function \(u(x)\) which is unaltered when moving from one lattice point to another is called a Bloch function \([u(x) = u(x+Na)]\).

**Bloch's theorem**

\[
\psi_k = \sum_n e^{ikna} \phi_n
\]

(a solution of the Schrödinger equation)

\[
\psi_k = \sum_n \{(\cos kna + isinkna)\phi_n\}
\]

Elementary Band Theory for Extended Solids

\[
\psi_k = \sum_n \{(\cos kna + isinkna)\phi_n\}
\]

\[
\psi(k) = \sum_n e^{inka} \phi_n
\]

1-dimensional case

- 1-D Brillouin zone from \(-a^*/2\) to \(a^*/2\)
- \(a^* = 2\pi/a\)
- \(-\pi/a \leq k \leq \pi/a\)

Consider \(k = 0\): zone center \(\Gamma\)
\[
\cos(kna) = \cos(0) = 1
\]
\[
\sin(kna) = \sin(0) = 0
\]
\[
\psi = \sum \phi_n = \phi_0 + \phi_1 + \phi_2 + \phi_3 + \ldots
\]

Consider \(k = \pi/a\): zone border \(X\)
\[
\cos(kna) = \cos(n\pi) = (-1)^n
\]
\[
\sin(kna) = \sin(n\pi) = 0
\]
\[
\psi = \sum (-1)^n\phi_n = \phi_0 - \phi_1 + \phi_2 - \phi_3 + \ldots
\]
Elementary Band Theory for Extended Solids

**Example: linear infinite chain of equidistant H atoms**

**Zone center \( \Gamma \)**

\[ \psi = \sum \phi_n = \phi_0 + \phi_1 + \phi_2 + \phi_3 + \ldots \]

- All in phase;
- All bonding (\( \sigma \))

**Zone border X**

\[ \psi = \sum (-1)^n \phi_n = \phi_0 - \phi_1 + \phi_2 - \phi_3 + \ldots \]

- All out of phase;
- All antibonding (\( \sigma^* \))

Plot \( E \) as a function of \( k \):

\[ -\pi/a \leq k \leq \pi/a; \]

\[ E(k) = E(-k) \]

**Other case: s, p and d orbitals in an infinite chain.**

Let \( z \) be in the chain direction. Then, \( p_x \) will be analog to \( p_y \) and \( d_{xz} \) to \( d_{x^2-y^2} \) and \( d_{yz} \) to \( d_{xy} \).

**Zone center \( \Gamma \)**

\[ \psi = \sum \phi_n = \phi_0 + \phi_1 + \phi_2 + \phi_3 + \ldots \]

- All in phase; but ? bonding ?

**Zone border X**

\[ \psi = \sum (-1)^n \phi_n = \phi_0 - \phi_1 + \phi_2 - \phi_3 + \ldots \]

- All out of phase; but ? bonding ?

Bonding/antibonding: depends on in phase/out of phase AND orientation
How to calculate $E(k)$?

$$\psi (k) = \sum_n e^{inka} \phi_n$$

Crystal Schrodinger Equation: $H\psi(k) = E(k)\psi(k)$

$$E(k) = \frac{<\psi^*(k)\hat{H}\psi(k)>}{<\psi^*(k)\psi(k)>}$$

$<\phi^*_m|\phi_n> = 1\ldots (m = n)$

$<\phi^*_m|\phi_n> = 0\ldots (m \neq n)$

$<\psi^*(k)|\psi(k)> = \sum_{m,n} <\phi^*_m|\phi_n> = N$
\[ \psi(\mathbf{k}) = \sum_n e^{i \mathbf{k} \cdot \mathbf{a}_n} \phi_n \]

\[ < \psi^*(\mathbf{k}) | \hat{H} | \psi(\mathbf{k}) > \]

1. \( m=n \)

\[ < \psi^*(\mathbf{k}) | \hat{H} | \psi(\mathbf{k}) > = \sum_n < \phi^*_n | \hat{H} | \phi_n > = N\alpha \]

2. \( m\neq n \), consider only the nearest neighbor

\[ < \phi^*_n | \hat{H} | \phi_{n\pm 1} > = \beta \]

\[ E(\mathbf{k}) = \frac{< \psi^*(\mathbf{k}) | \hat{H} | \psi(\mathbf{k}) >}{< \psi^*(\mathbf{k}) | \psi(\mathbf{k}) >} \]

\[ = \frac{N\alpha + N\beta (e^{i \mathbf{k} \cdot \mathbf{a}} + e^{-i \mathbf{k} \cdot \mathbf{a}})}{N} \]

\[ = \alpha + 2\beta \cos \mathbf{k} \cdot \mathbf{a} \]

\[ E(\mathbf{k}) = \left\langle e^{-i \mathbf{k} \cdot \mathbf{a}_n} | \hat{H} | \left\{ e^{i \mathbf{k} \cdot (n-1) \mathbf{a}} \phi_{n-1} + e^{i \mathbf{k} \cdot n \mathbf{a}} \phi_n + e^{i \mathbf{k} \cdot (n+1) \mathbf{a}} \phi_{n+1} \right\} \right\rangle \]

\[ = \alpha + 2\beta \cos \mathbf{k} \cdot \mathbf{a} \]
**Elementary Band Theory for Extended Solids**

Densities of states (DOS)

\( \Delta E \) number of levels in the energy interval \( \Delta E \)

\[ \alpha - 2\beta \]

\[ \alpha + 2\beta \]

DOS is proportional to the inverse slope of the band:

- steep bands (large overlap) \( \Rightarrow \) small DOS
- flat bands (small overlap) \( \Rightarrow \) large DOS

**DOS\( (E_F) \) determines properties**

- e.g., electrical conductivity, magnetic susceptibility, specific heat...

\[ \text{DOS}(E_F) = 0: \text{always nonmetallic} \]

\[ \text{DOS}(E_F) > 0: \text{often metallic} \]

---

**Elementary Band Theory for Extended Solids**

**Bandwidth (dispersion)**

The difference between highest and lowest level of one band.

The bandwidth is determined by the overlap between the interacting orbitals.

The smaller the distance between the atoms, the larger the bandwidth.

\[ 4\beta \]

Infinite chain of H atoms.