Section 8
Brillouin Zone and Reciprocal Lattice

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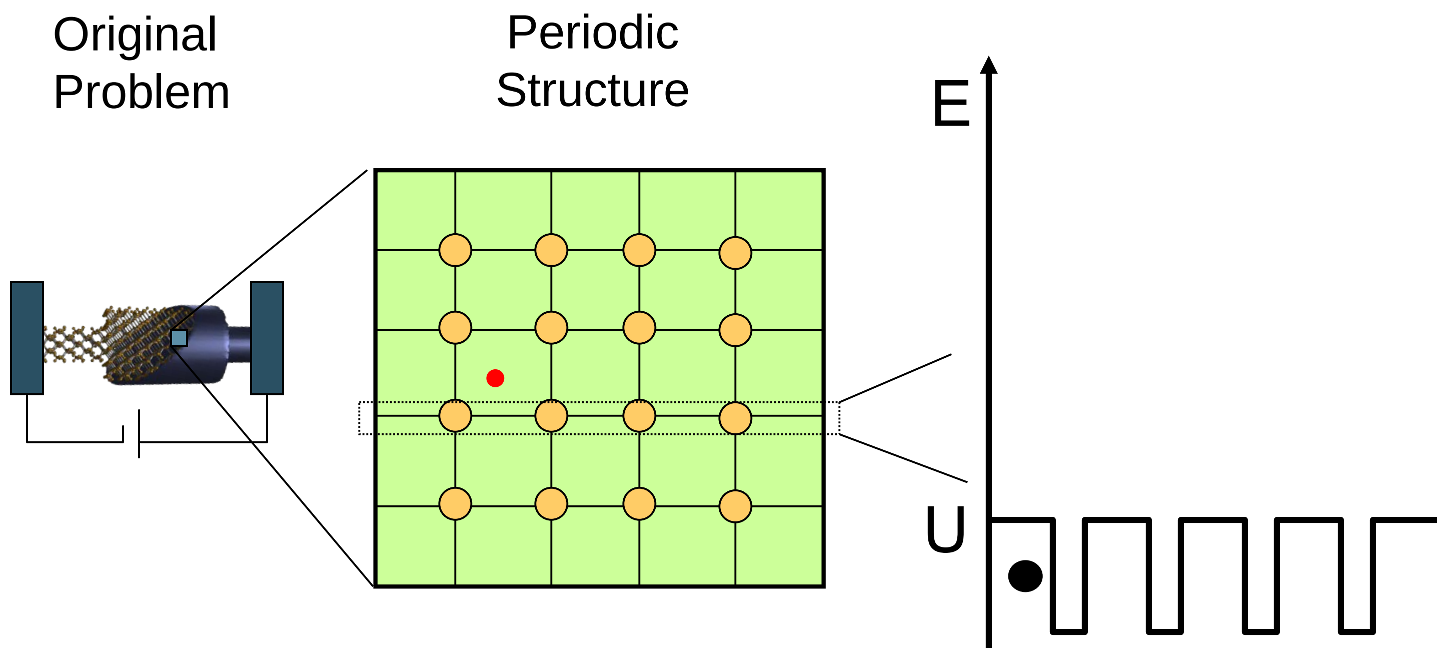
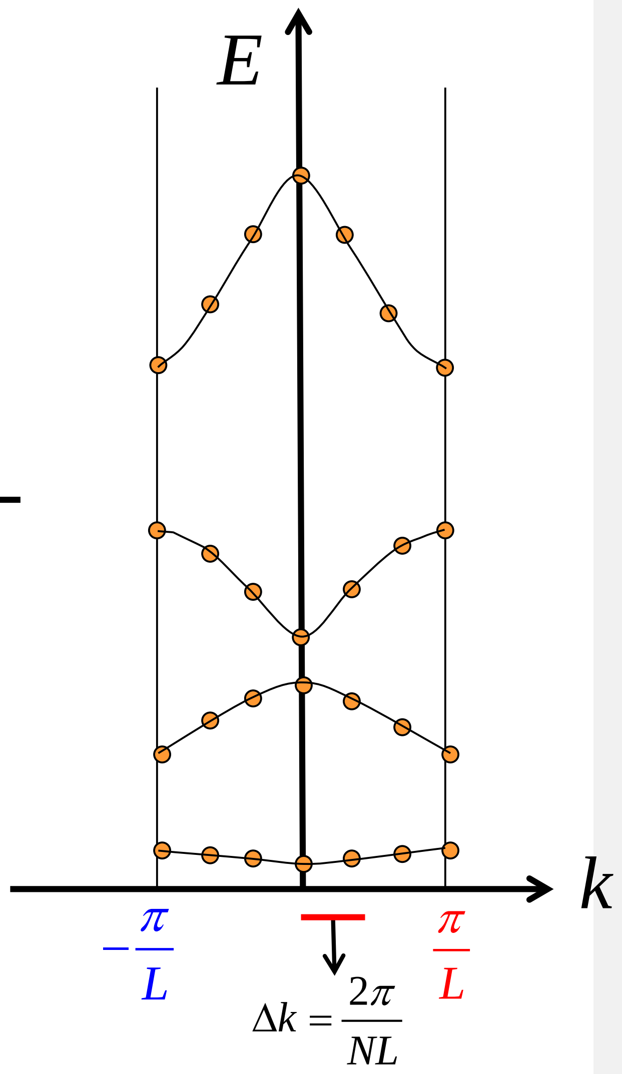




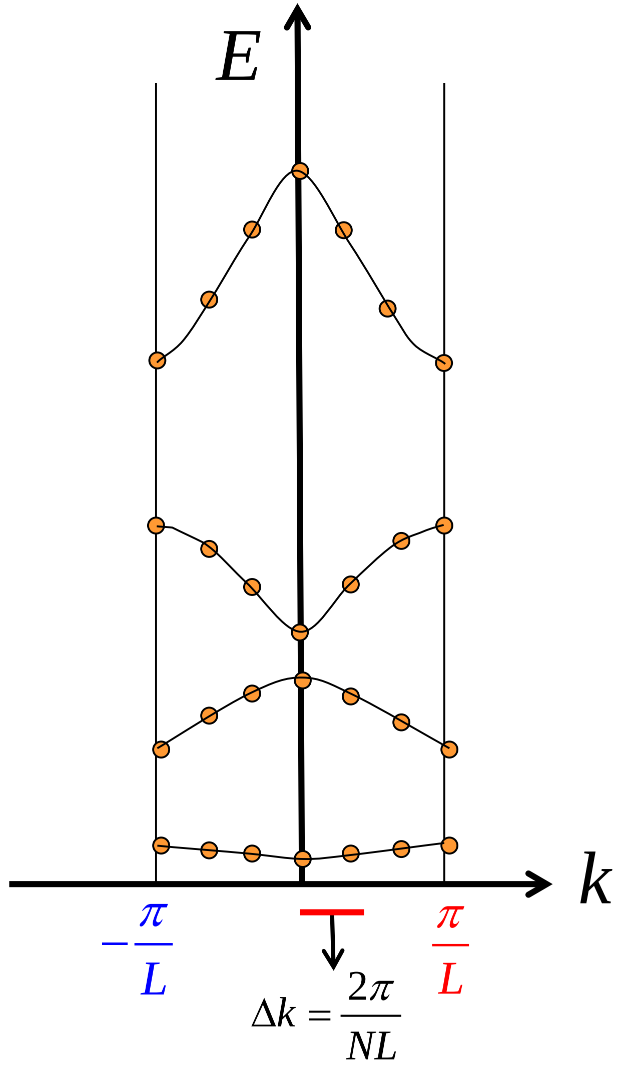
Section 7 – Bandstructure in 1D Periodic Potentials

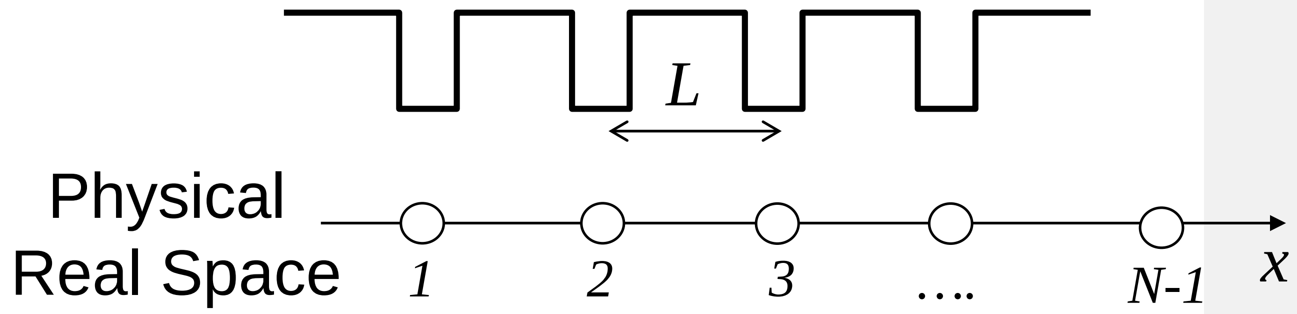
- 8.1 1D Brillouin Zone - Reciprocal Lattice
- 8.2 2D
- 8.3 3D

Reference: Vol. 6, Ch. 3

Daniel Mejia, Gerhard Klimeck (2019), "Periodic Potential Lab - Kronig Penney Model, " https://nanohub.org/resources/kronigpenneylab. (DOI: 10.21981/TT2Y-A185).

1D Brillouin Zone and Number of States





$$\psi[x+NL] = \psi(x)e^{ikLN} = \psi(x)e^{ikLN}e^{i2\pi m}$$

$$= \psi(x)e^{ikLN}e^{imkL}$$

$$k = \pm\frac{2\pi n}{NL} \quad n = -\frac{N}{2}.....-1,0,1,....\frac{N}{2}$$

$$\frac{States}{band} = \frac{k_{max} - k_{min}}{\Delta k} = \frac{2\pi/L}{2\pi/NL} = N$$

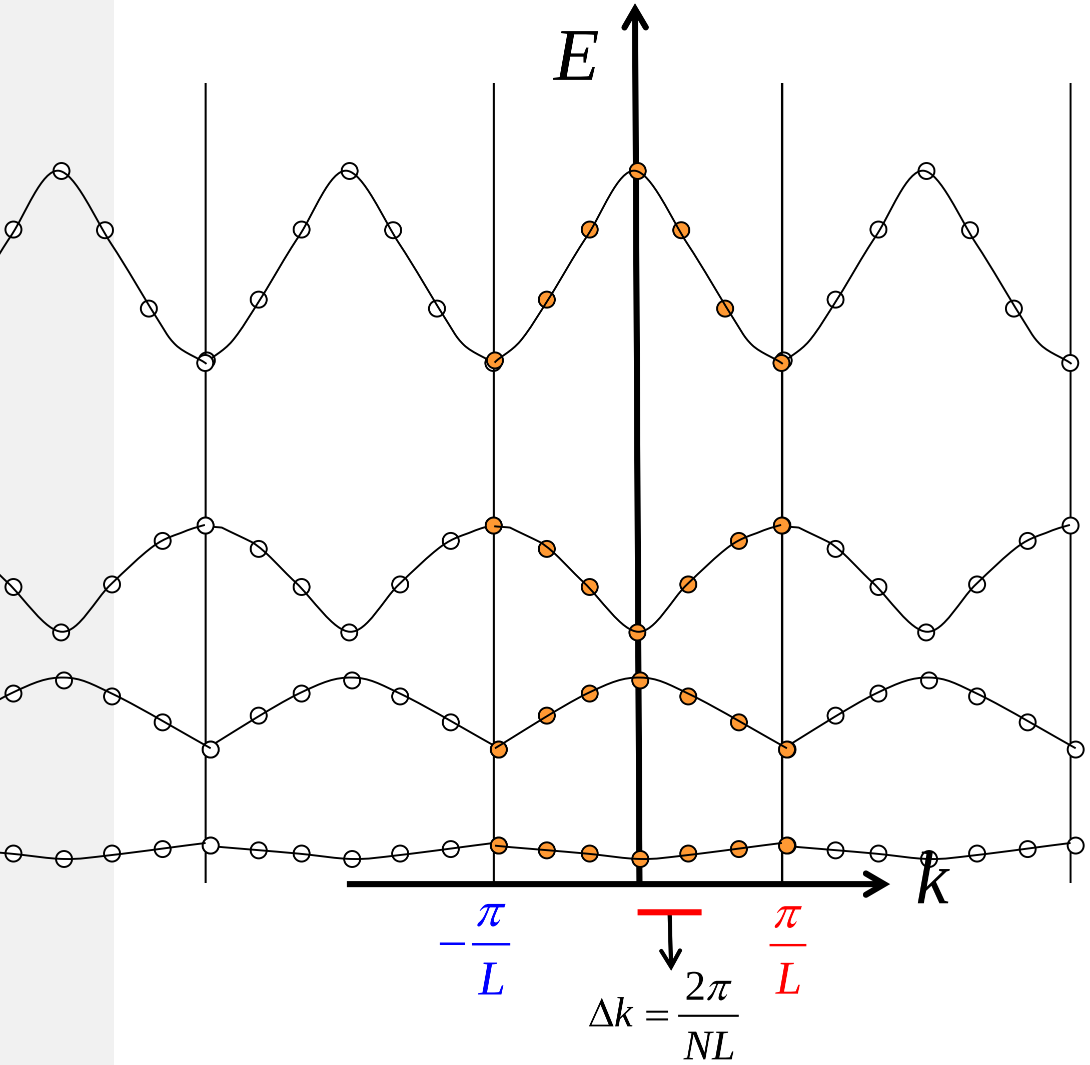
4 states per atom, N atoms

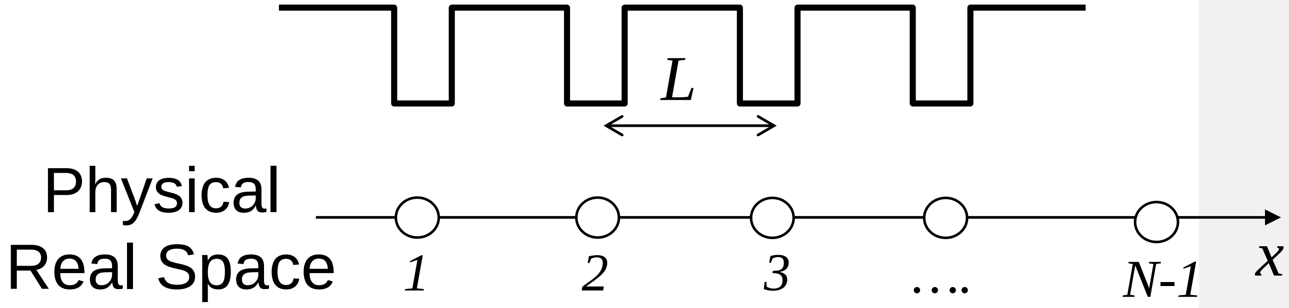
=> 4 bands, N states in each band

All states are included in the first zone

Invariant to shift by $1 = e^{im2\pi} = e^{imkL}$

1D Brillouin Zone and Number of States





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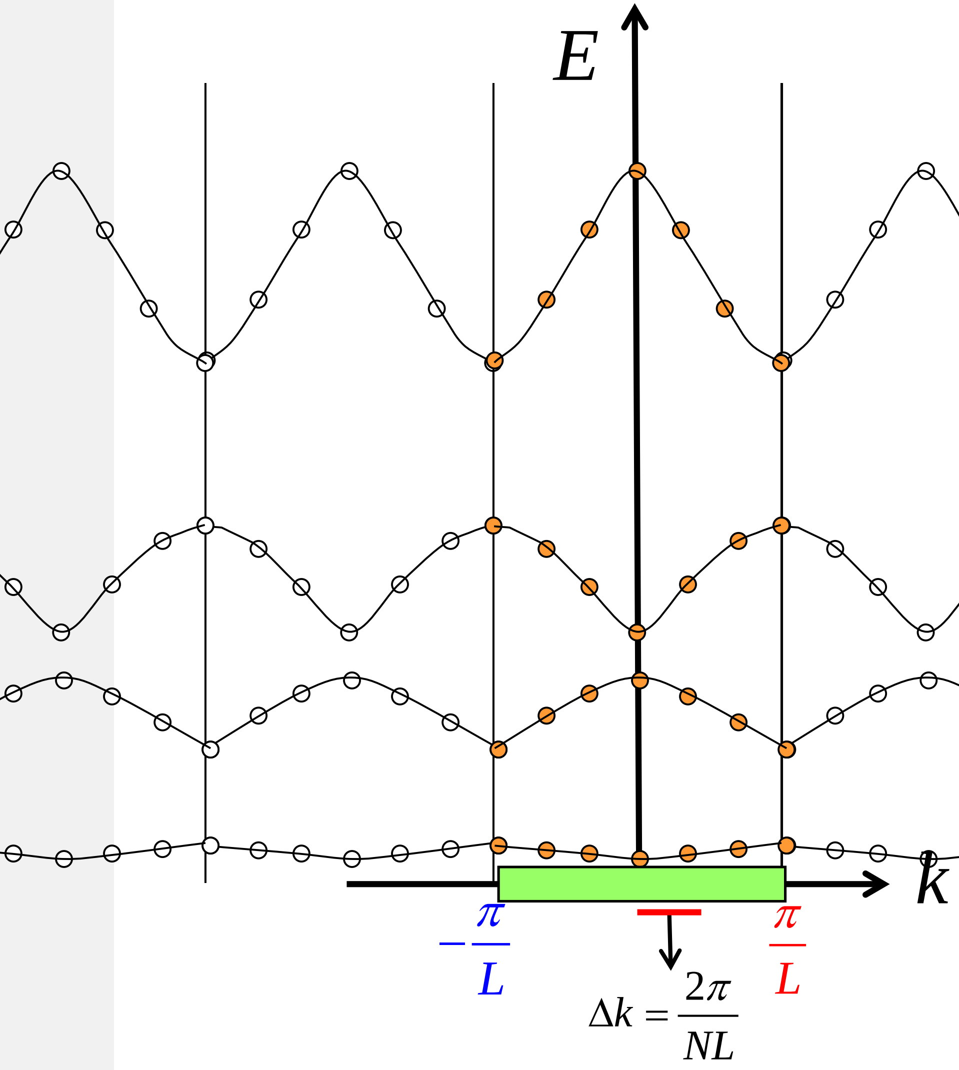
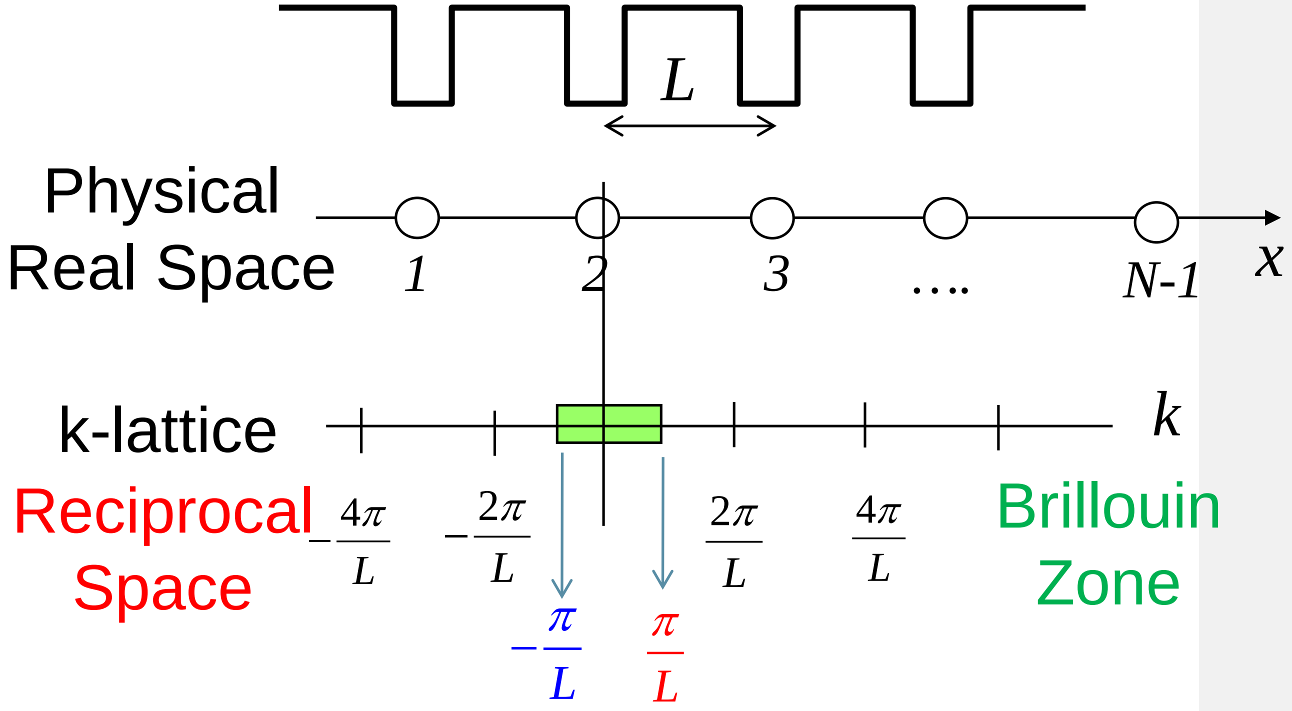
1D Brillouin Zone and Number of States





Collapse of a periodic (infinite) space into a discrete space

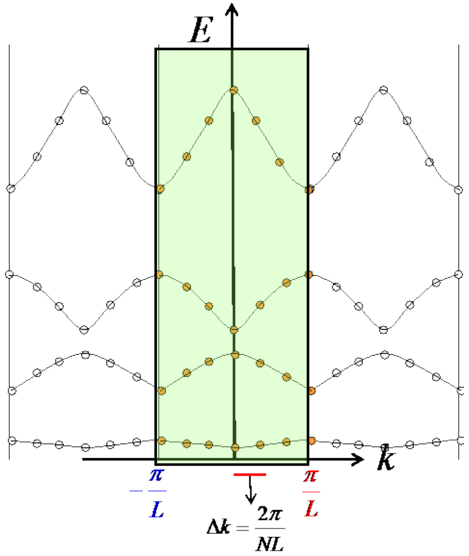
4 states per atom, N atoms
=> 4 bands, N states in each band
All states are included in the first zone
Invariant to shift by $1 = e^{im2\pi} = e^{imkL}$

Fourier Transform Reminders

$f(x)$	$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x)e^{-i\omega x}\,dx$	**Space Mapping**
1	$\sqrt{2\pi}\cdot\delta(\omega)$	
e^{iax}	$\sqrt{2\pi}\cdot\delta(\omega-a)$	**Periodic => discrete**
$\cos(ax)$	$\sqrt{2\pi}\cdot\frac{\delta(\omega-a)+\delta(\omega+a)}{2}$	**Collapse of a periodic (infinite) space into a discrete space**
$\mathrm{rect}(ax)$	$\frac{1}{\sqrt{2\pi a^2}}\cdot\mathrm{sinc}\left(\frac{\omega}{2\pi a}\right)$	
$\mathrm{tri}(ax)$	$\frac{1}{\sqrt{2\pi a^2}}\cdot\mathrm{sinc}^2\left(\frac{\omega}{2\pi a}\right)$	**finite <=> infinite**
$e^{-a\|x\|}$	$\sqrt{\frac{2}{\pi}}\cdot\frac{a}{a^2+\omega^2}$	
$e^{-\alpha x^2}$	$\frac{1}{\sqrt{2\alpha}}\cdot e^{-\frac{\omega^2}{4\alpha}}$	**infinite <=> infinite**

Critical Conceptual Steps

- Basis State Selection
  - » Physical problem is based on a 1D/2D/3D periodic array of atoms
  - » Desired system/signal response is periodic in space
  - » Physical space is infinitely extended
    - ✓ Can the physical space be collapsed into a different representation?
  - » Chose a basis system of plane waves
  - » New finite reciprocal space is representative of the original system
- Solution of the Schrödinger Equation
  - » Solution with plane waves in reciprocal space
  - » 1D solution performed in Kronig-Penney model (last Section 7)
    - ✓ Band formation



$$f(\boldsymbol{r}) = f(\boldsymbol{r} + \boldsymbol{R}_n)$$

$$\sum_m f_m e^{i\mathbf{G}_m \cdot \mathbf{r}} = f(\mathbf{r})$$

Collapse of a periodic (infinite) space into a discrete space

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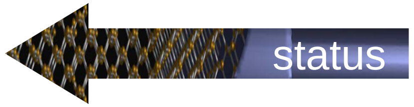
One Video Segment

- 8.1 1D Problems
  - » Brillouin Zone
  - » Solution strategy
  - » Reciprocal Lattice

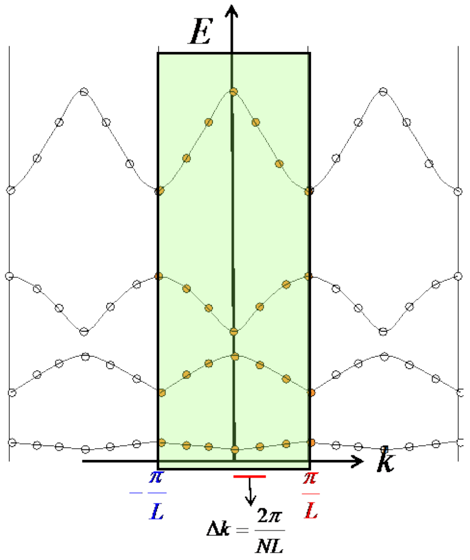


One Video Segment

- 8.2 2D Problems

One Video Segment

- 8.3 3D Problems



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Prasad Sarangapani, Arun Goud Akkala, Sebastian Steiger, Hong-Hyun Park, Yosef Borga, Tillmann Christoph Kubis, Michael Povolotskyi, Gerhard Klimeck (2014), "Brillouin Zone Viewer," https://nanohub.org/resources/brillouin. (DOI: 10.4231/D3DB7VQ35).

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One Video Segment

- 8.1 1D Problems
  - » Brillouin Zone
  - » Solution strategy
  - » Reciprocal Lattice

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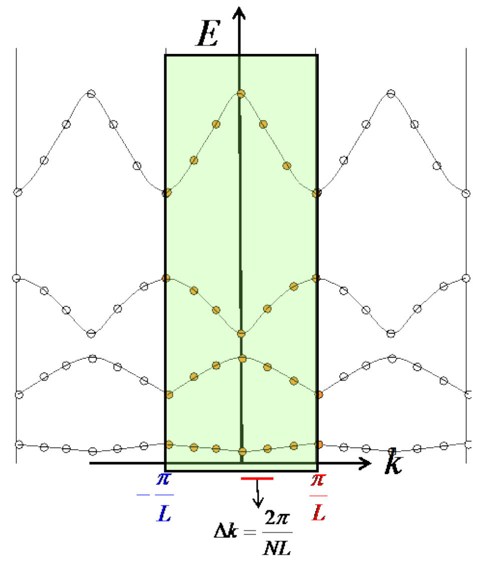
One Video Segment

- 8.2 2D Problems
  - » Reciprocal Lattice Recipe
  - » Examples - Square and Hexagonal

One Video Segment

- 8.3 3D Problems



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