Section 7
Bandstructure in 1D Periodic Potentials
7.2 Bandstructure - Solutions

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Section 7
Bandstructure - in 1D Periodic Potentials

One Video Segment

- 7.1 Bandstructure - Problem Formulation
  - » Kronig-Penney Model setup
  - » Bloch theorem
  - » Analytical solution process

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

$$\frac{1-2\xi}{2\xi\sqrt{1-\xi}}\times\ldots\ldots\ldots\ldots=\cos kL \qquad \xi\equiv\frac{E}{U_0} \qquad \alpha_0\equiv\sqrt{\frac{2mU_0}{\hbar^2}}$$

One Video Segment

- 7.2 Bandstructure - Solutions

status

  - » Bandgaps
  - » Comparison to finite system model

$$\frac{1-2\xi}{2\xi\sqrt{1-\xi}}\times\ldots\ldots\ldots\ldots=\cos kL$$

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

One Video Segment

- 7.3 Band Properties

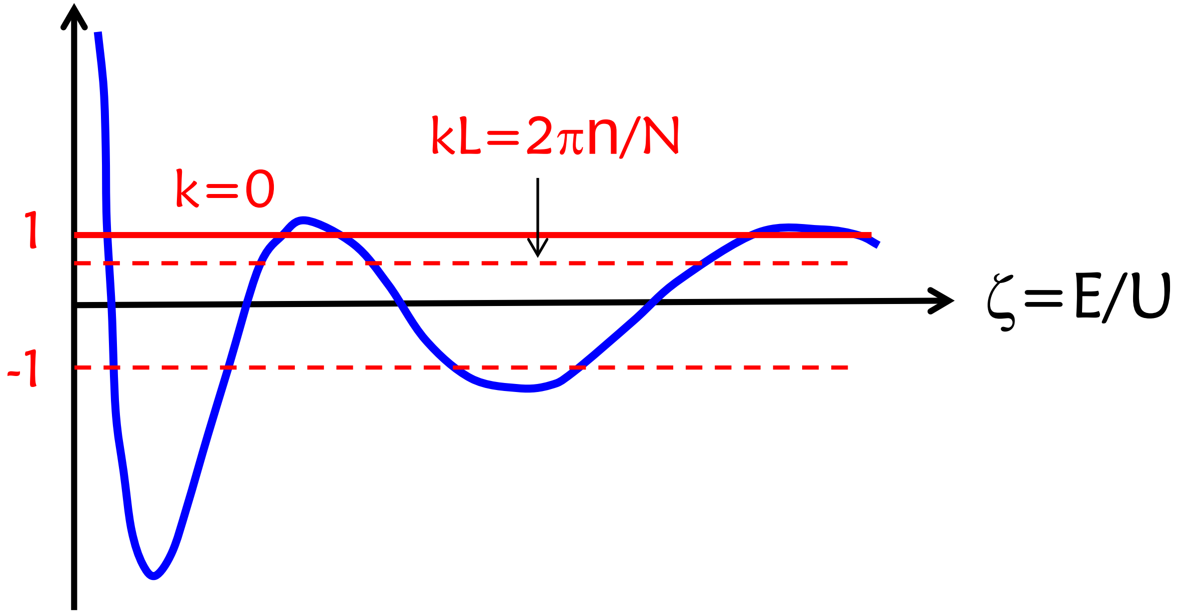
Reference: Vol. 6, Ch. 3

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

Graphical solution to Energy Levels

$$\frac{1-2\xi}{2\xi\sqrt{1-\xi}} \times \ldots\ldots\ldots\ldots = \cos kL$$

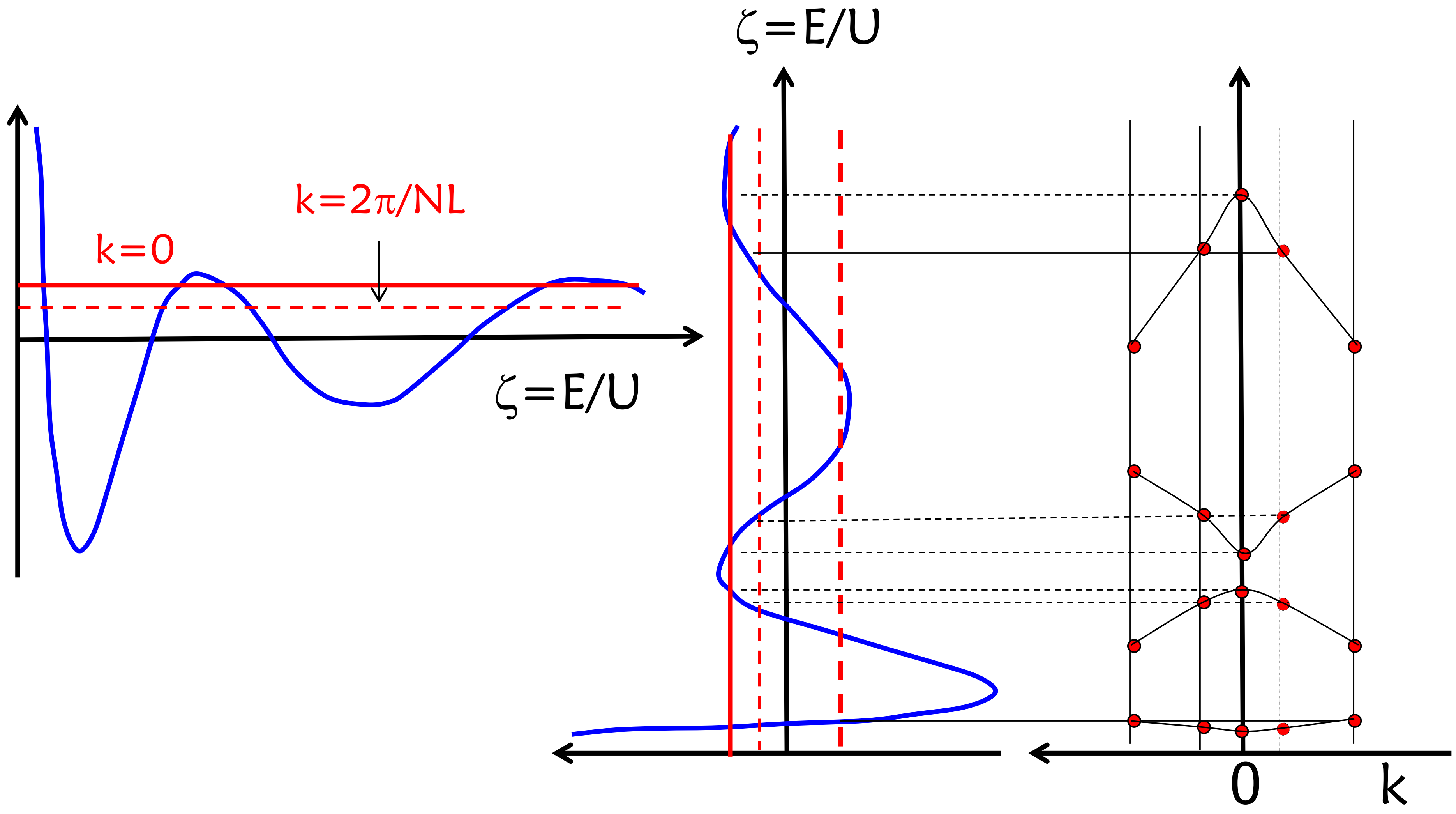
$$k = \pm\frac{2\pi n}{NL} \qquad n = -\frac{N}{2}\ldots\ldots -1, 0, 1, \ldots\frac{N}{2}$$



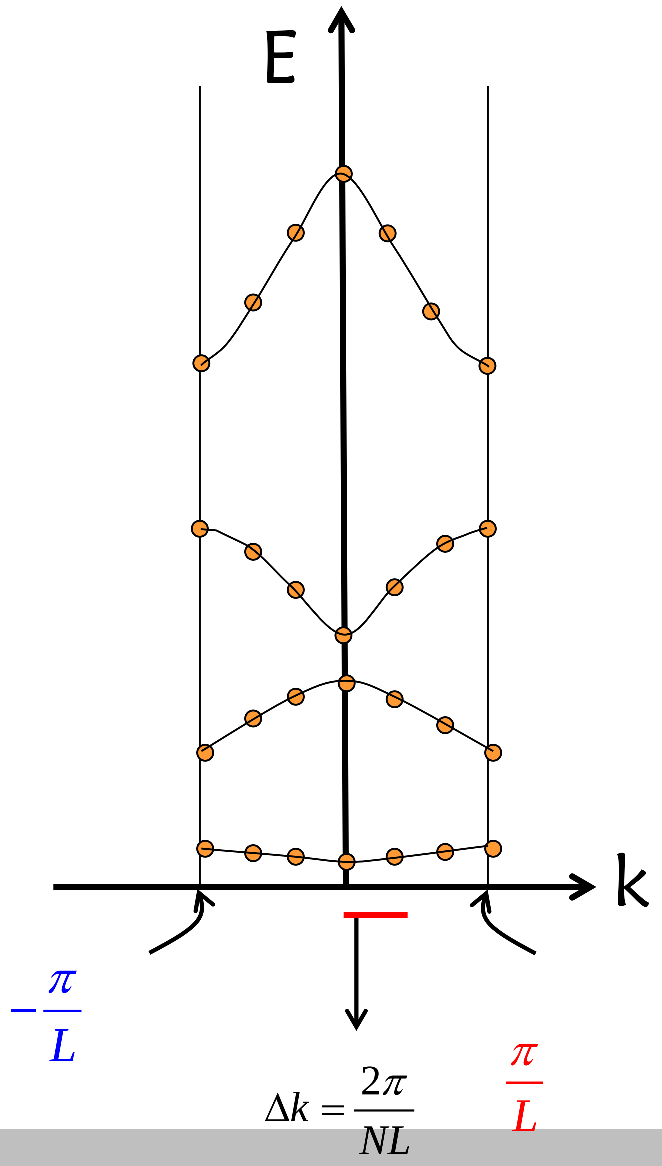
Right Hand side is a set of N flat lines between -1 and 1

Left Hand side is an ocilatory function with damping

Energy Band Diagram



Brillouin Zone and Number of States

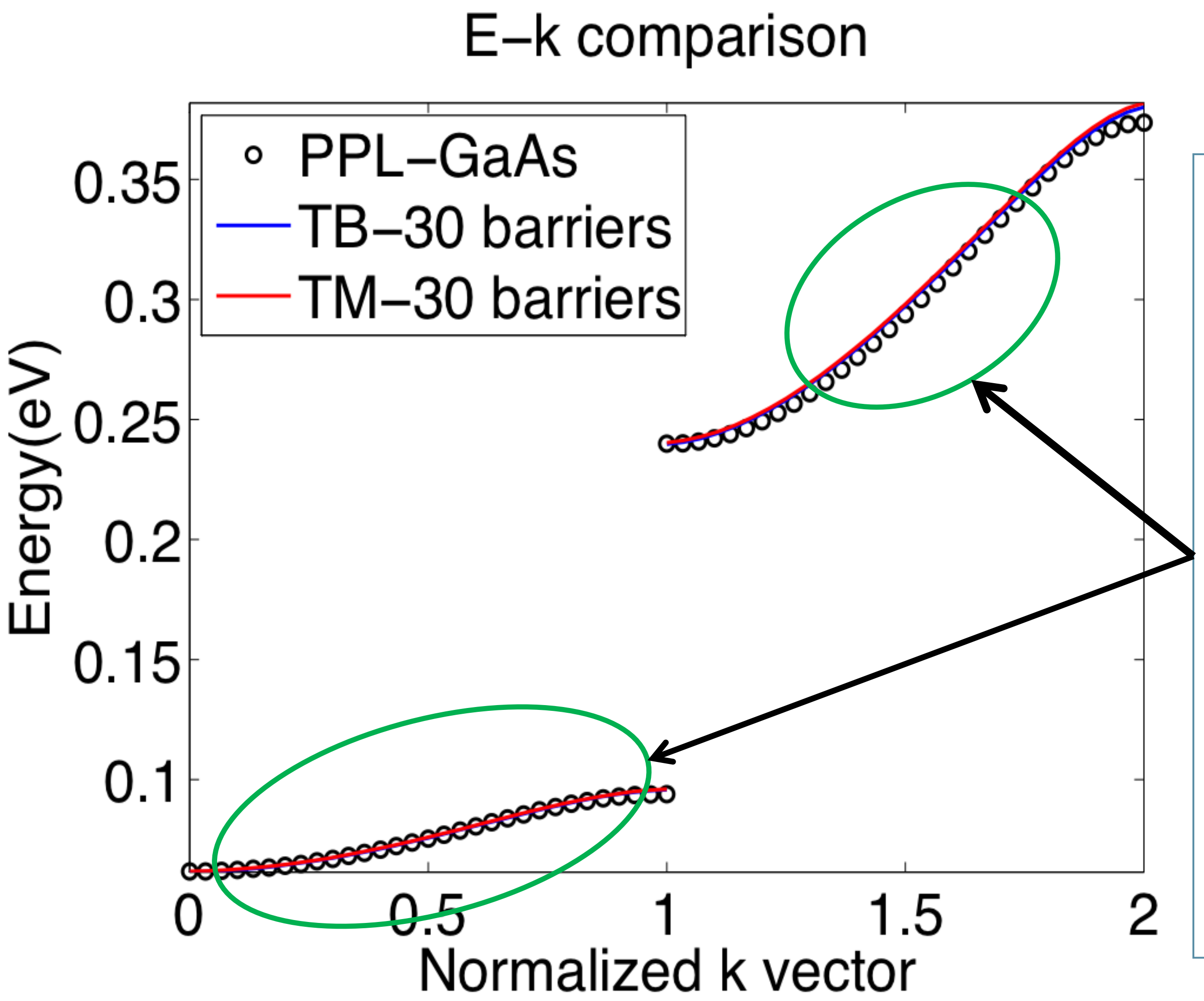


$$k = \pm\frac{2\pi n}{NL} \quad n = -\frac{N}{2}.....-1,0,1,....\frac{N}{2}$$

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

4 states per atom, N atoms
=> 4 bands, N states in each band

GaAs Well Comparison - 30 Barriers

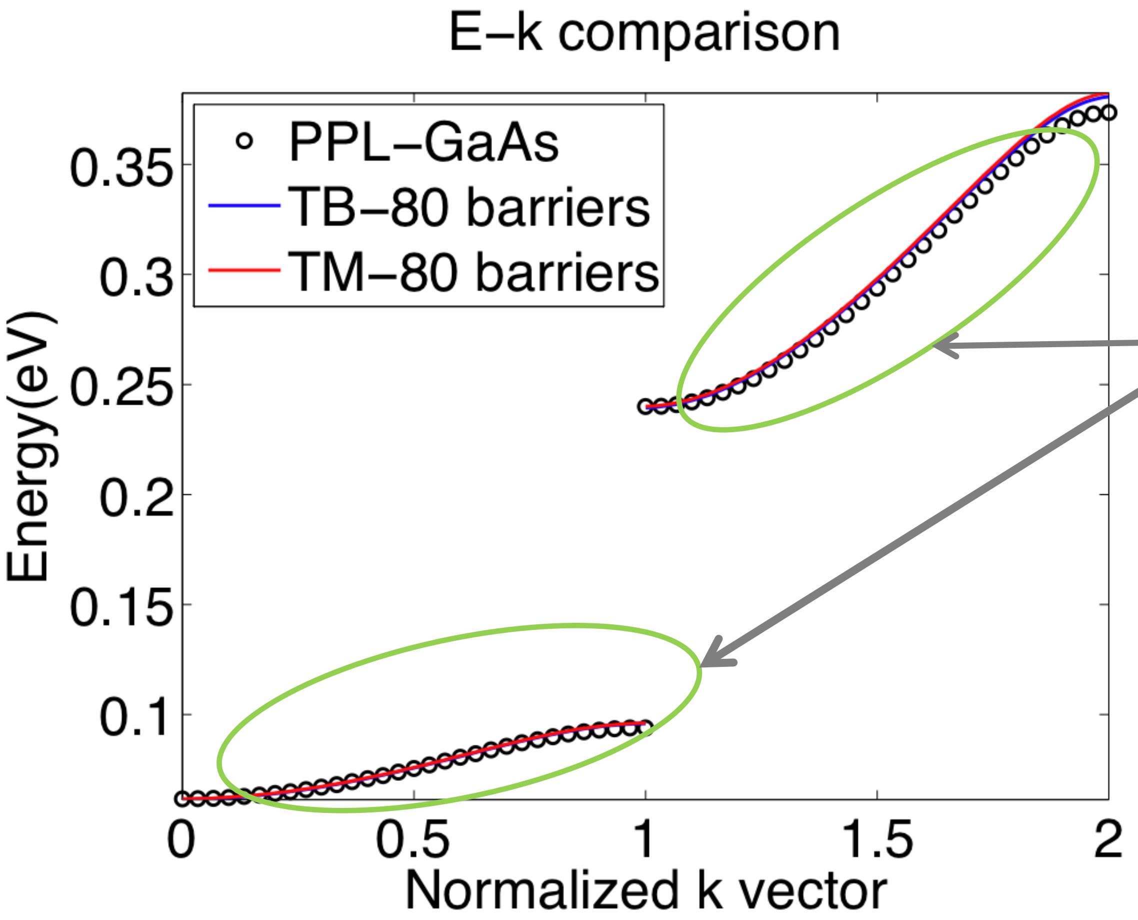


A GaAs structure with 6nm wells, 2nm barriers and 0.4eV barrier height is modeled as follows,

- PPL-Periodic structure repeated indefinitely.
- TB: 30 barriers using tight-binding.
- TM: 30 barriers using transfer matrices.

It can be seen that the results of these three approaches agree well.

GaAs Well Comparison - 80 Barriers



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- PPL-Periodic structure repeated indefinitely.
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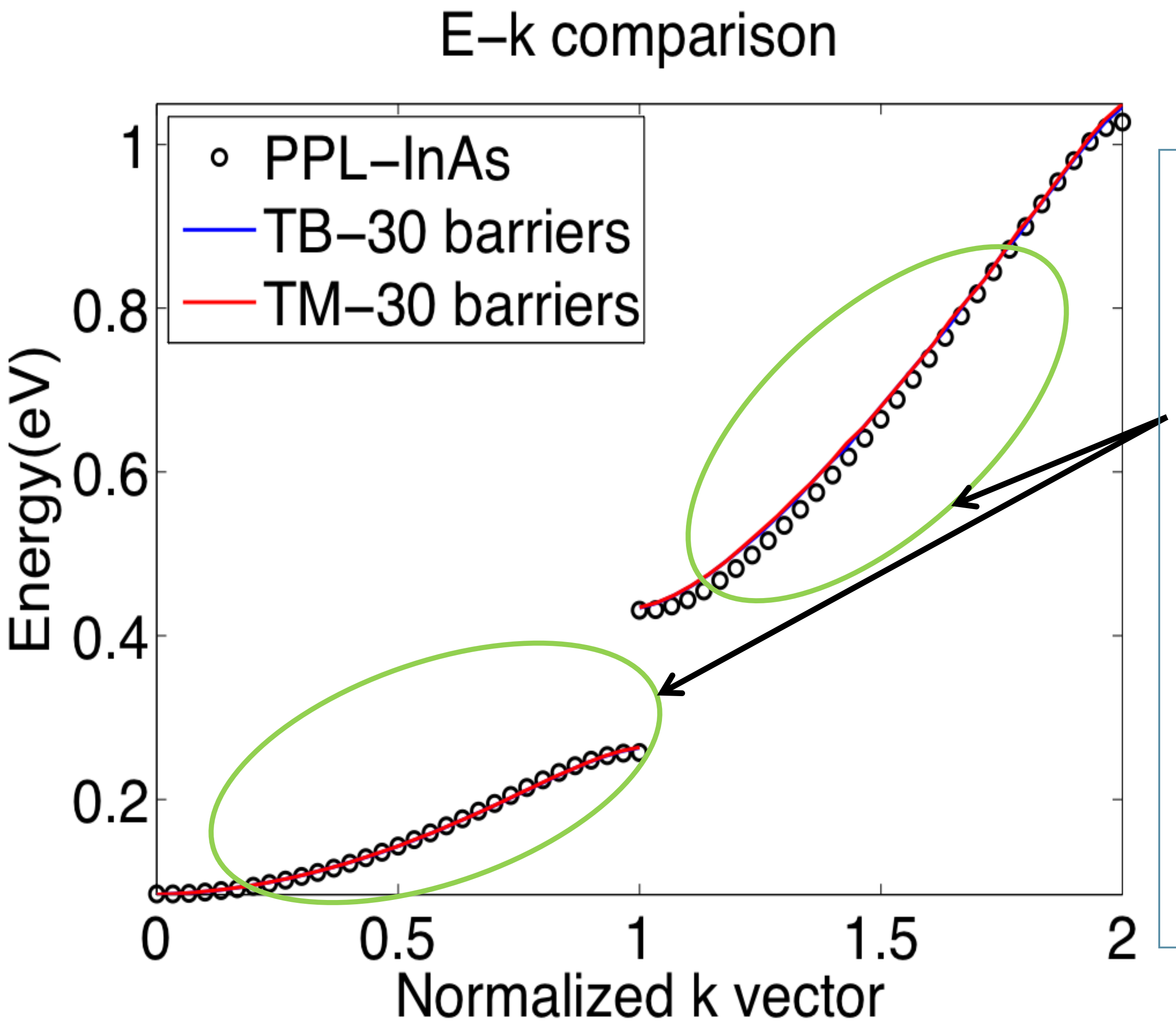
InAs Well Comparison - 30 Barriers



An InAs structure with 6nm wells, 2nm barriers and 0.4eV barrier height is modeled as follows,

- PPL-Periodic structure repeated indefinitely.
- TB: 30 barriers using tight-binding.
- TM: 30 barriers using transfer matrices.

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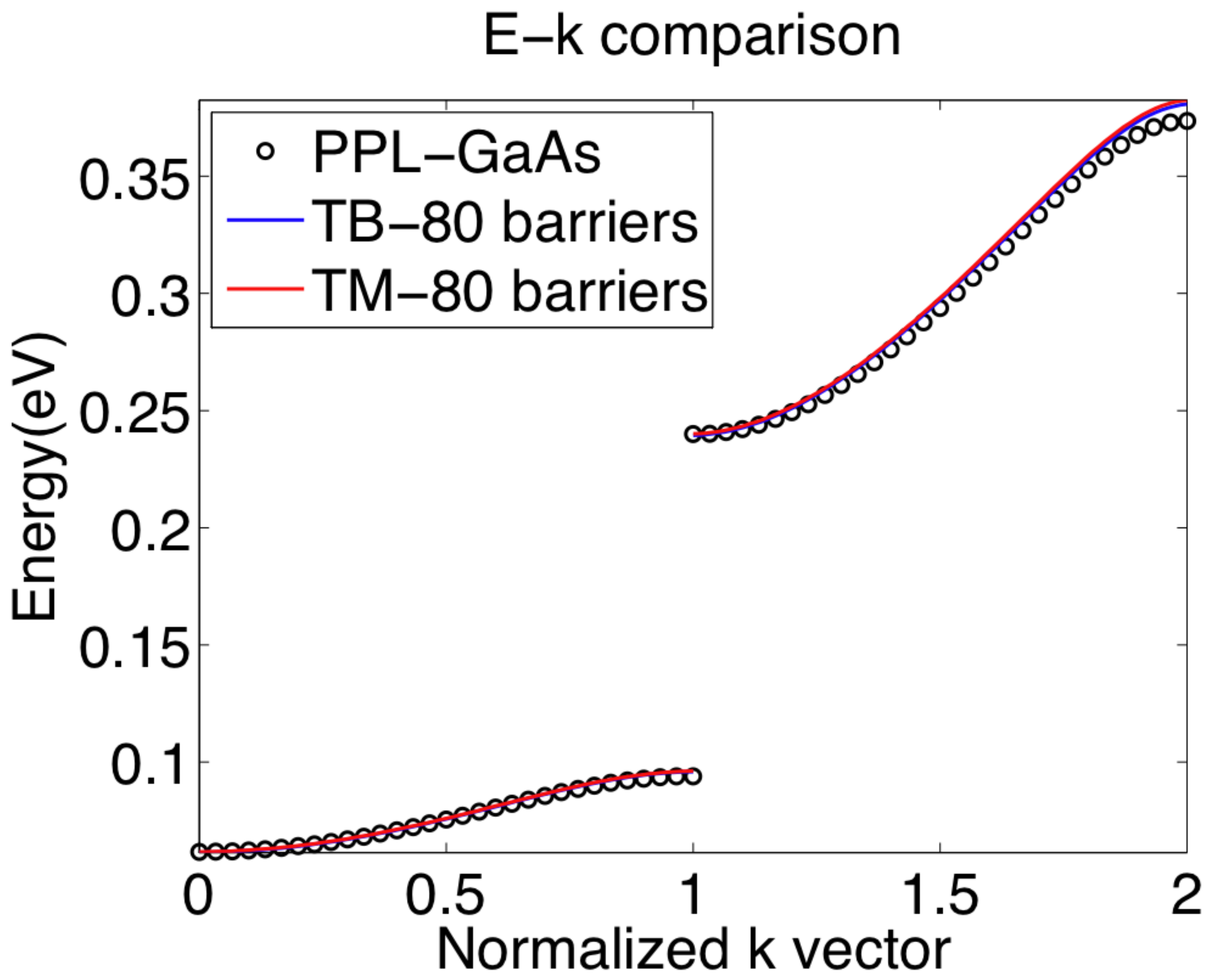
Key Summary

- Finite superlattice with large number of repeated cells approaches the periodic potential model



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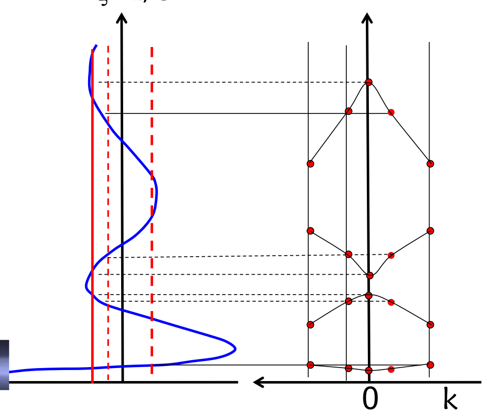
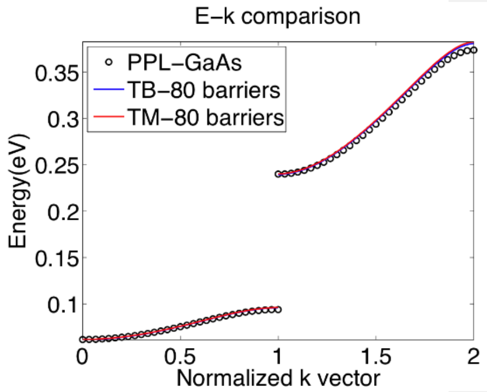
One Video Segment

- 7.2 Bandstructure - Solutions
  - » Bandgaps
  - » Comparison to finite system model

status





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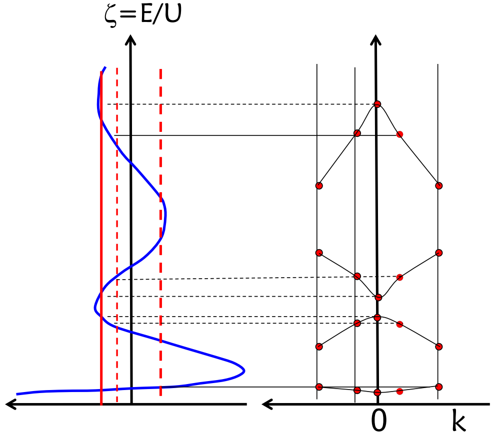

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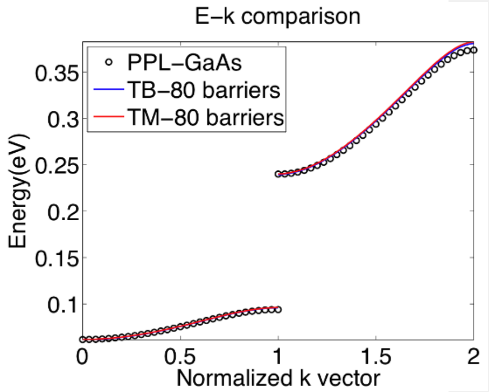

One Video Segment

- 7.3 Band Properties ← status
  - » Wave packets
  - » Effective mass
  - » Electrons and Holes

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