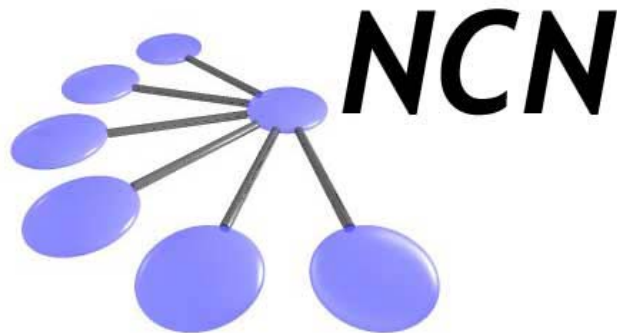


# Network for Computational Nanotechnology (NCN)

UC Berkeley, Univ. of Illinois, Norfolk State, Northwestern, Purdue, UTEP

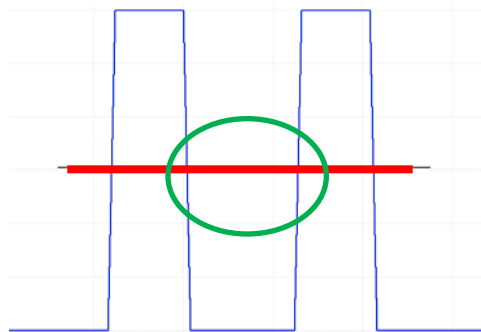
## Open 1D Systems: Formation of Bandstructure



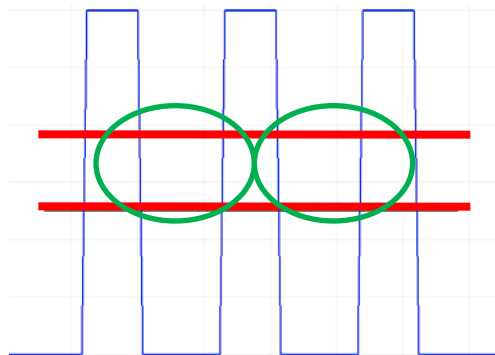
Gerhard Klimeck,  
Dragica Vasileska,  
Samarth Agarwal

**PURDUE**  
UNIVERSITY

# Reminder Transmission through Repeated wells

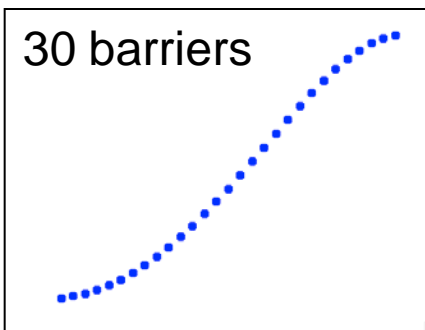
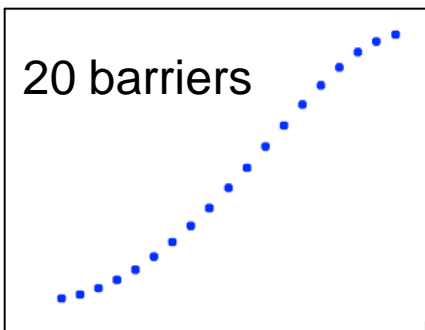
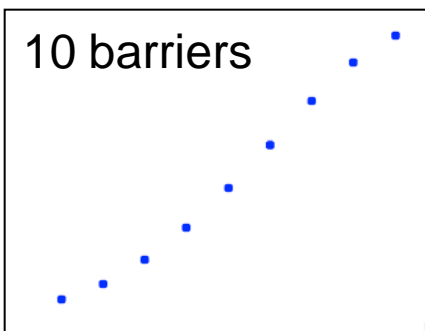


2 barriers => 1 resonance



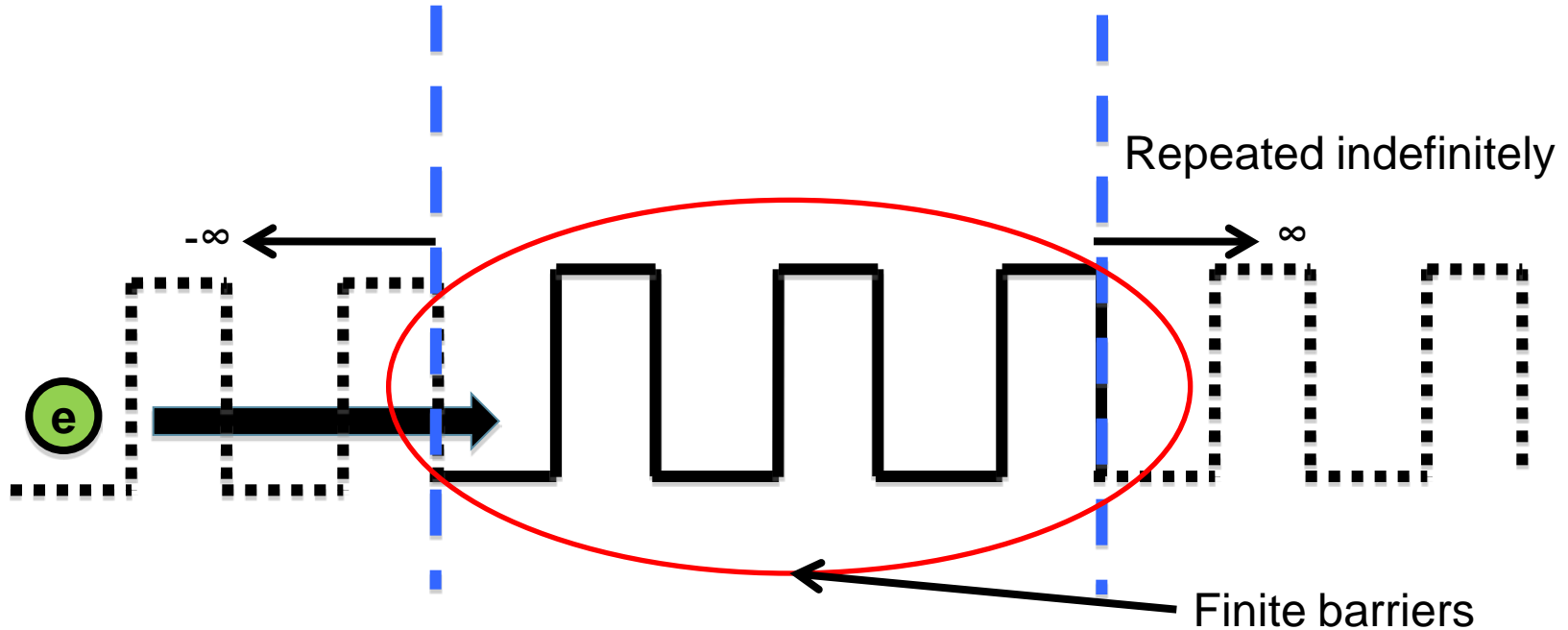
3 barriers => 2 resonance

n barriers => n-1 resonance



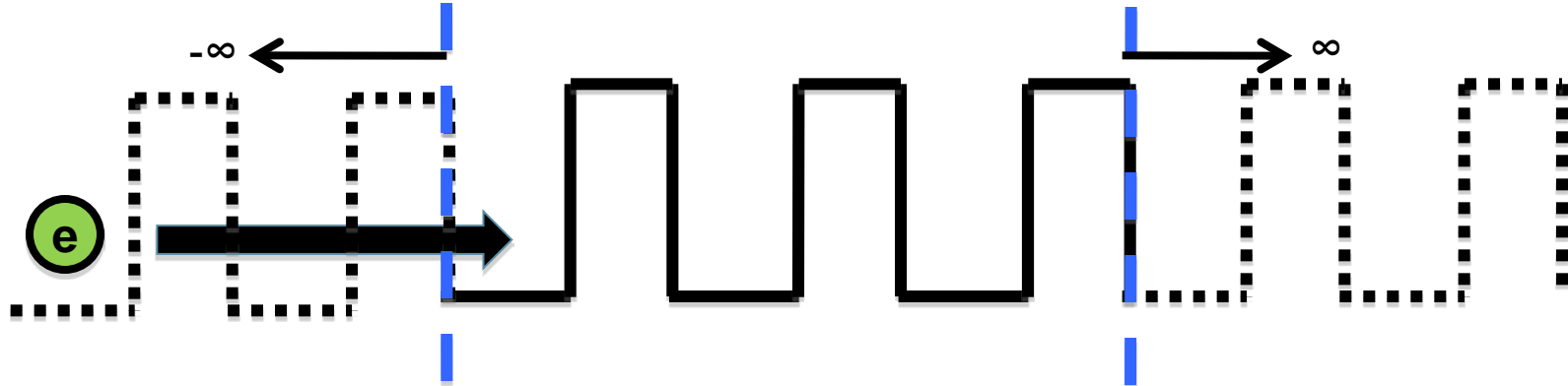
As the number of barriers are increased more and more energy resonances begin to appear and energy bands are formed.

# Comparison with Periodic structure



As the number of barriers is increased the electrons see no difference between the actual structure and a structure that is simply modeled as being repeated indefinitely (Periodic).

# The Kronig-Penney model



- Problem: Energy levels in a periodic potential.
- Solve: Schrodinger equation for a periodic potential.
- Bloch theorem: Wave-function for a periodic potential satisfies,

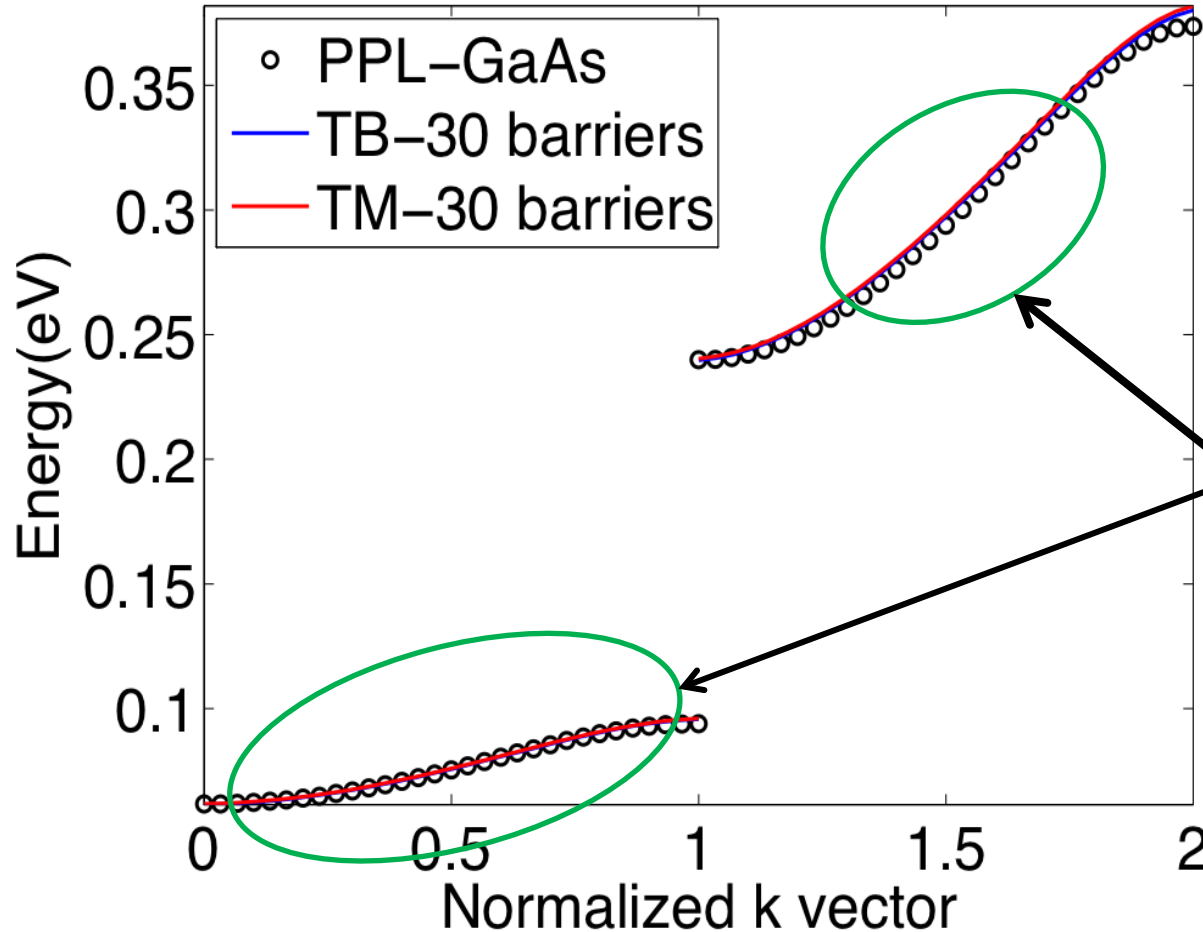
$$\psi(x + a) = e^{ika} \psi(x)$$

‘ $a$ ’: periodicity of the potential ‘ $k$ ’: wave-vector.

- Using the Bloch theorem the allowed energy levels in a given periodic potential can be found.
- This approach is referred to as the Kronig-Penney model.

# GaAs Well Comparison - 30 Barriers

## E-k comparison



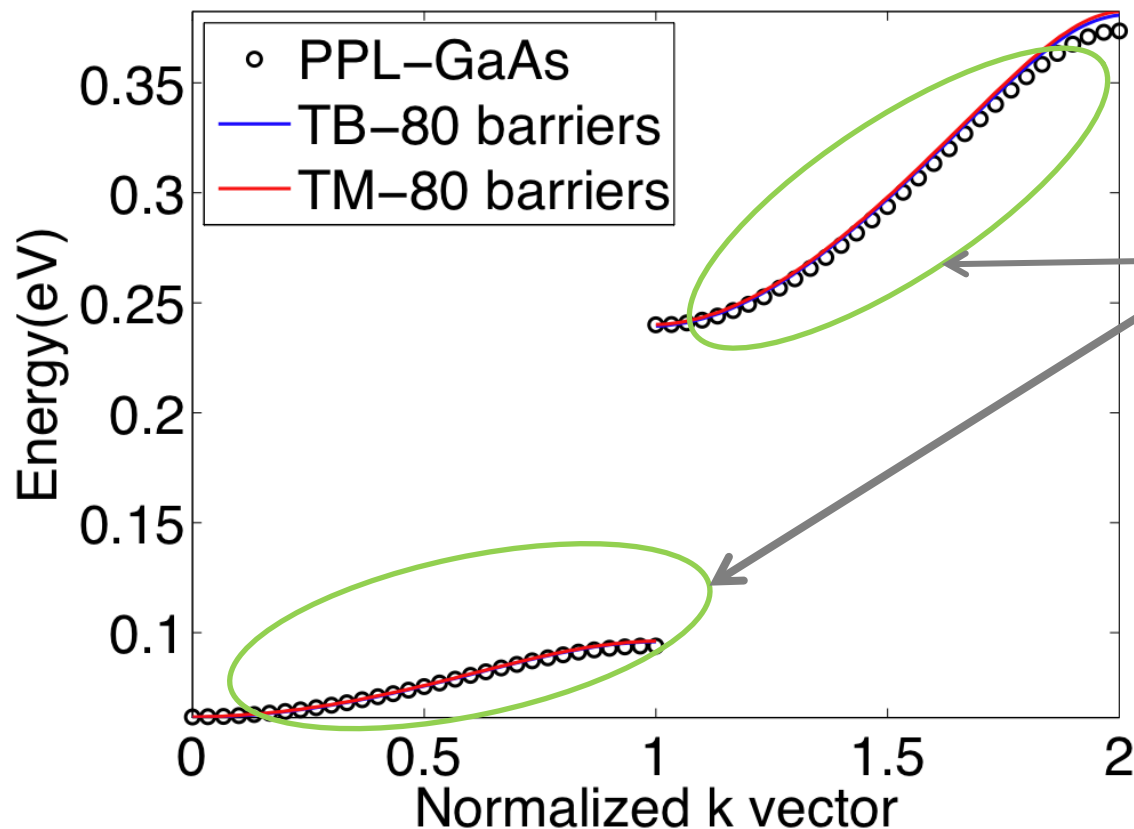
A GaAs structure with 6nm wells, 2nm barriers and 0.4eV barrier height is modeled as follows,

- 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

E-k comparison



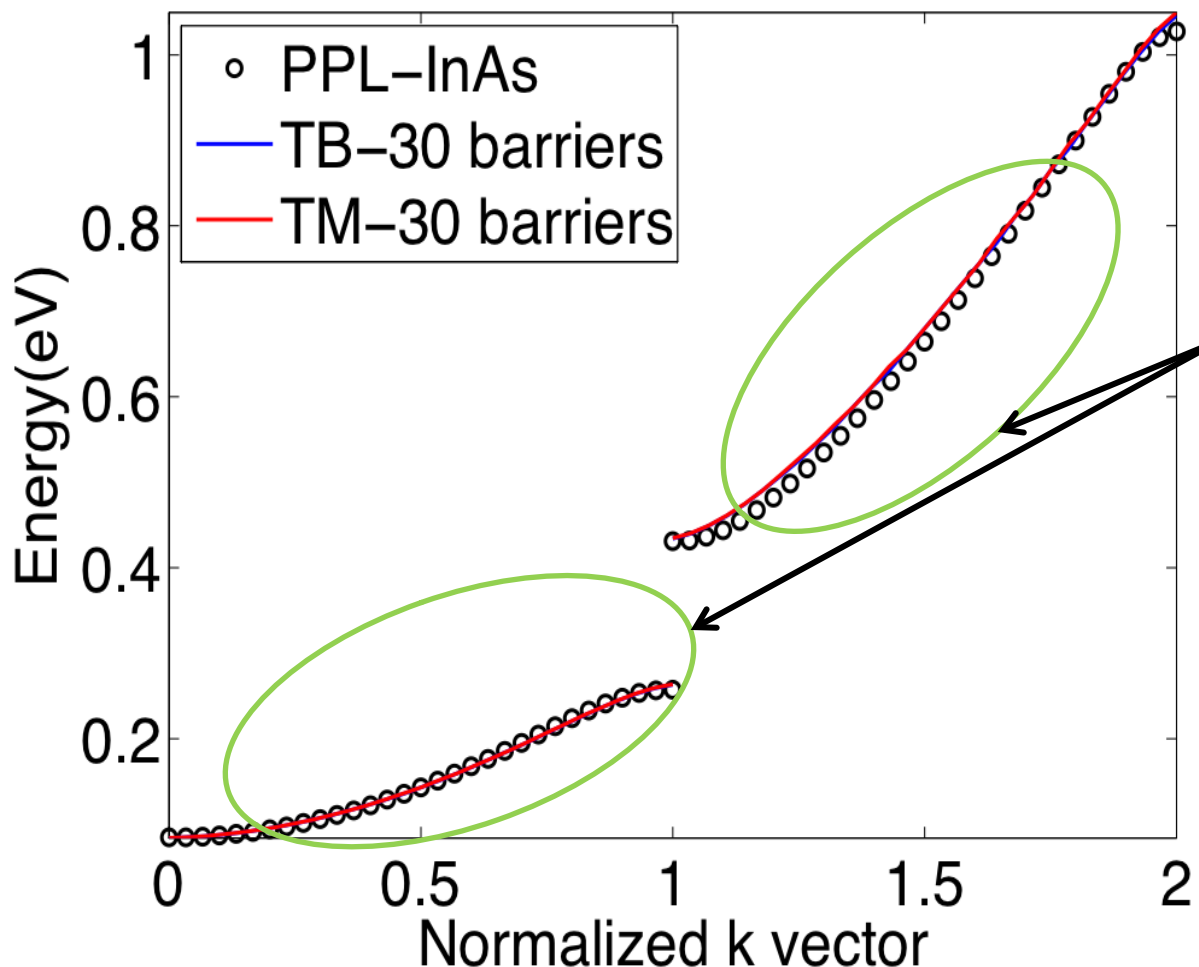
A GaAs structure with 6nm wells, 2nm barriers and 0.4eV barrier height is modeled as follows,

- PPL-Periodic structure repeated indefinitely.
- TB: 80 barriers using tight-binding.
- TM: 80 barriers using transfer matrices.

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

# InAs Well Comparison - 30 Barriers

## E-k comparison



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.

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

## Key Summary

- Finite superlattice with large number of repeated cells approaches the periodic potential model
- Transfer Matrix and effective mass tight binding give about the same result

E-k comparison

