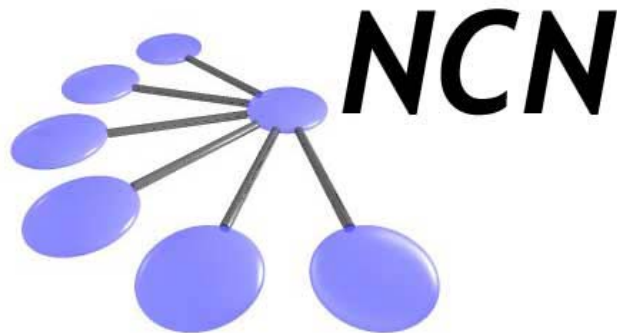


Network for Computational Nanotechnology (NCN)

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

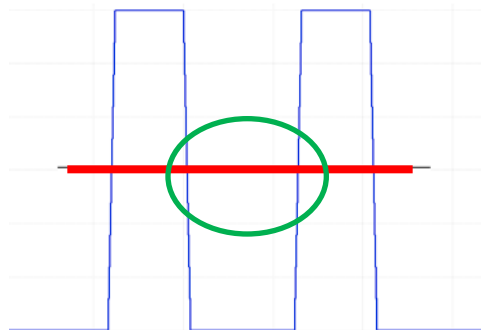
Open 1D Systems: Formation of Bandstructure



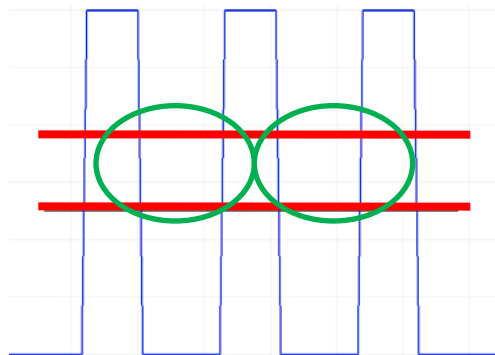
Gerhard Klimeck,
Dragica Vasileska,
Samarth Agarwal

PURDUE
UNIVERSITY

Reminder Transmission through Repeated wells

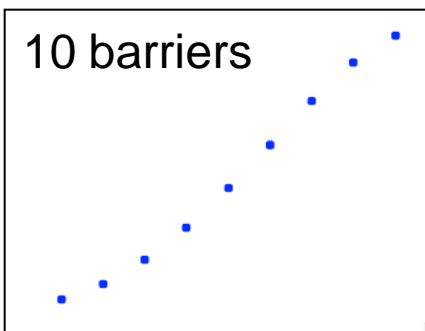


2 barriers => 1 resonance

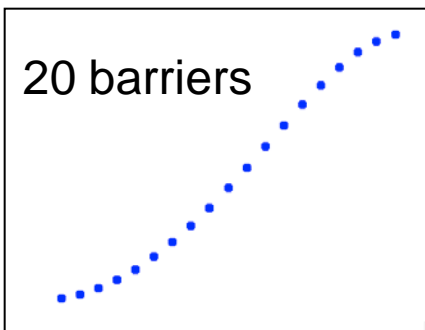


3 barriers => 2 resonance

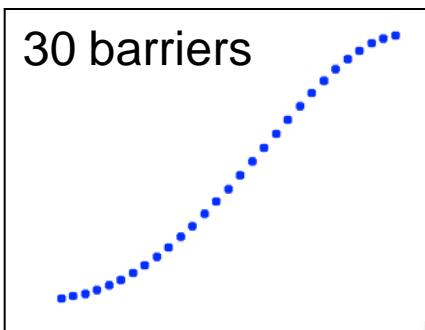
n barriers => n-1 resonance



10 barriers



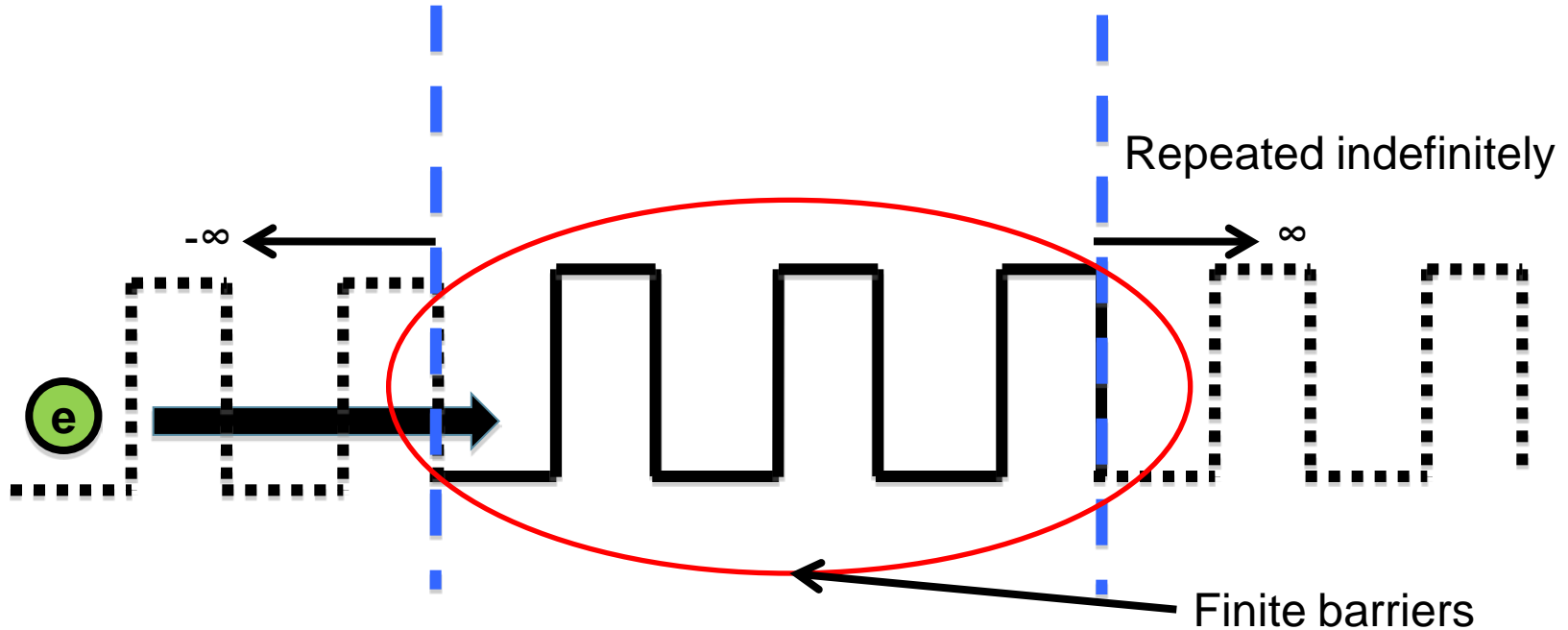
20 barriers



30 barriers

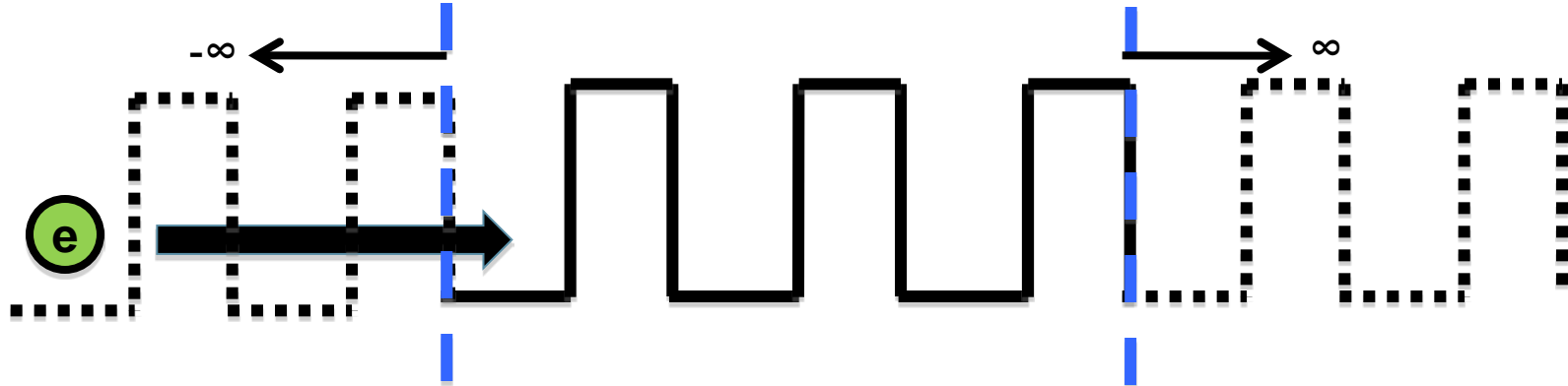
As the number of barriers are increased more and more energy resonances begin to appear and energy bands are formed.

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,

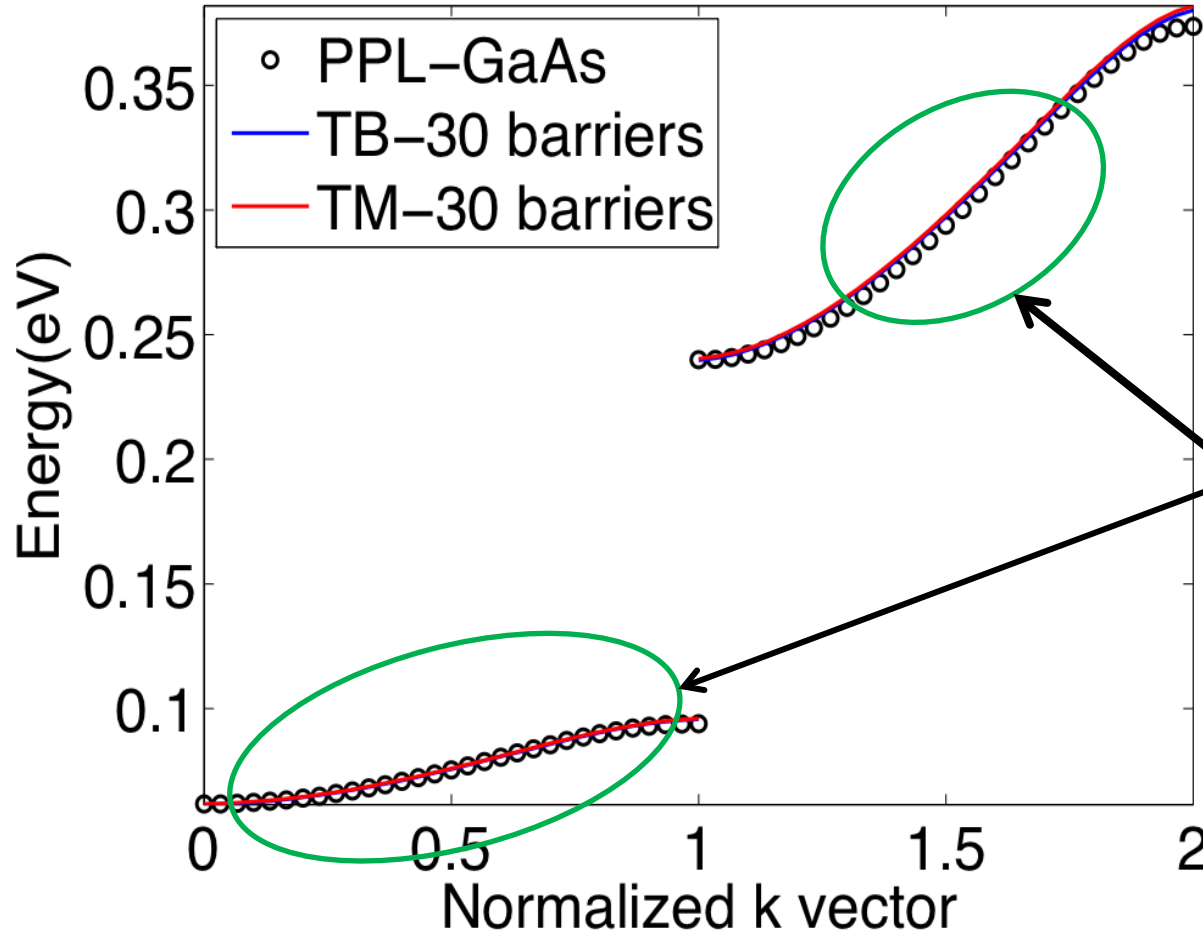
$$\psi(x + a) = e^{ika} \psi(x)$$

‘ 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



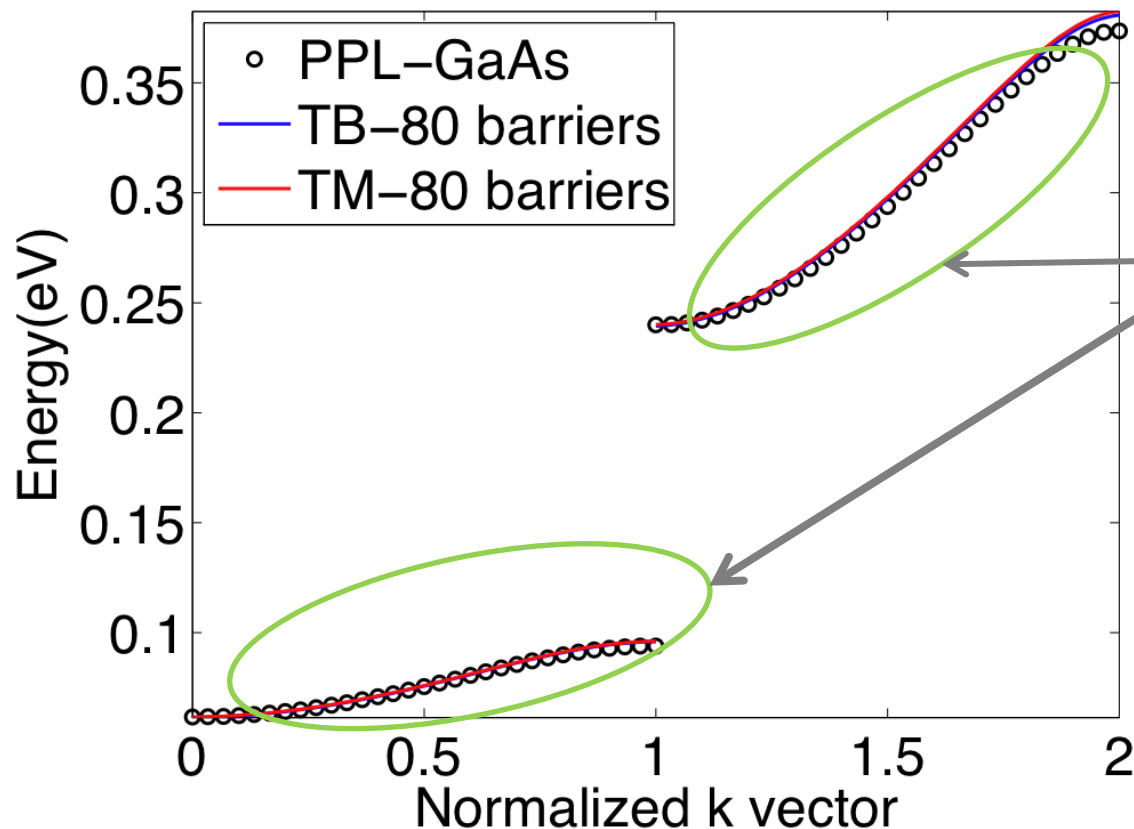
A GaAs structure with 6nm wells, 2nm barriers and 0.4eV barrier height is modeled as follows,

- 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



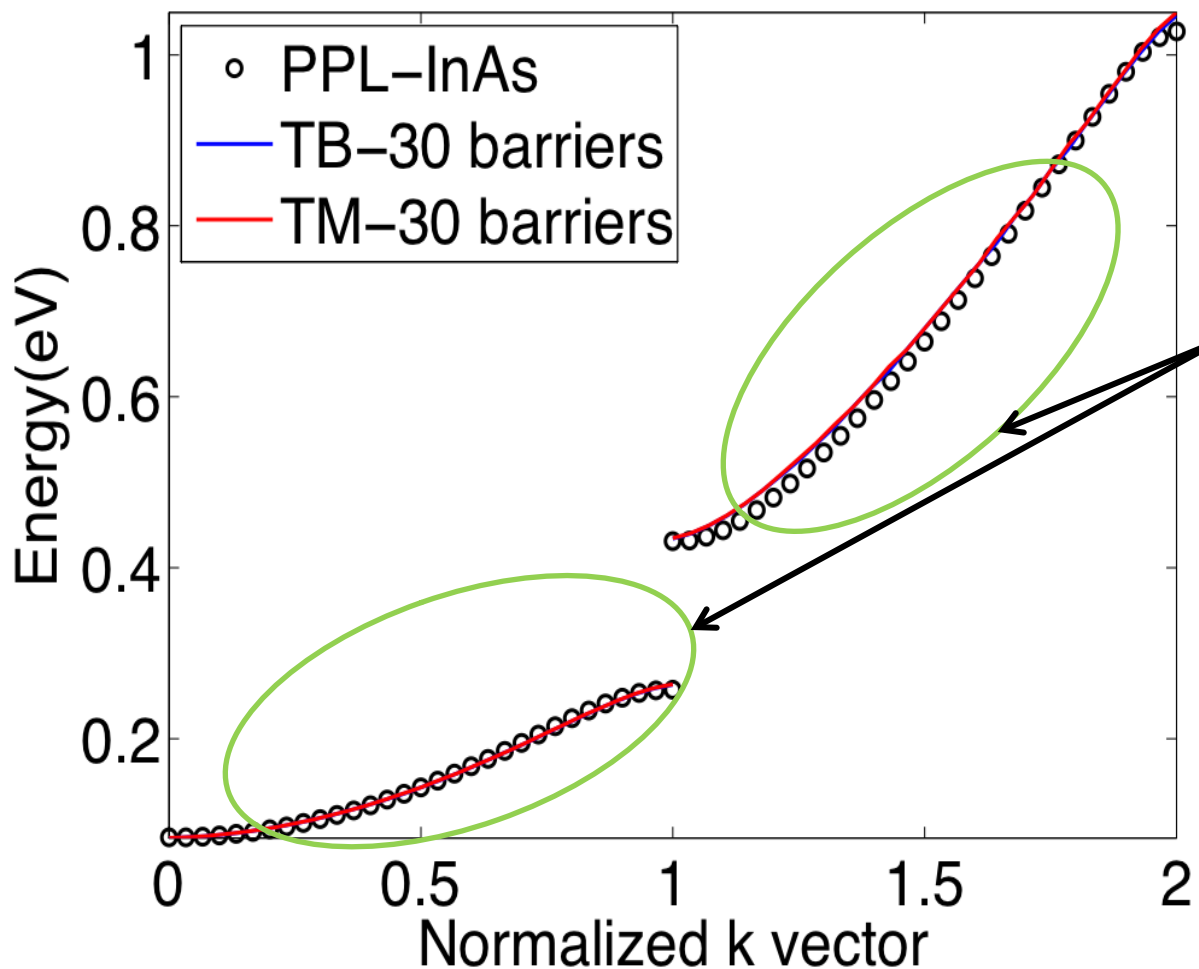
A GaAs structure with 6nm wells, 2nm barriers and 0.4eV barrier height is modeled as follows,

- 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

