Particles, atoms, and crystals 4

Coupled systems

Modern physics for engineers

David Miller

Coupled systems

Many systems in quantum mechanics are coupled, e.g.,

- atoms in molecules
- atoms in crystals

Detailed calculations of such systems can be complicated

- but behaviors can be seen
  - in a "coupled well"
    - by considering the first two energy levels

Coupled well

Consider

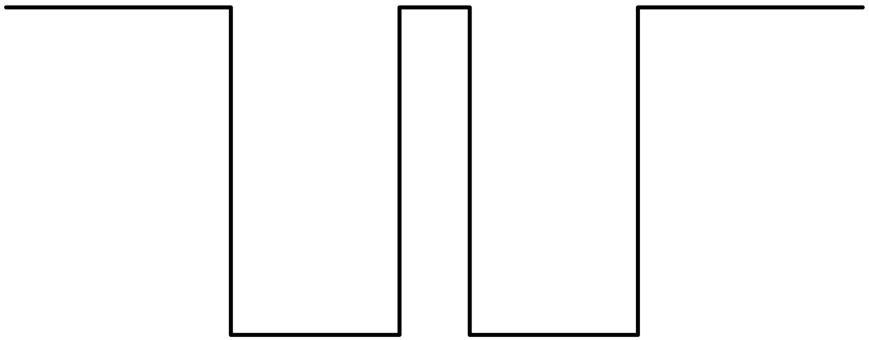
a pair of wells

both the same thickness

with finite height barriers

of arbitrarily large thickness on either side

and a specific thickness in the middle



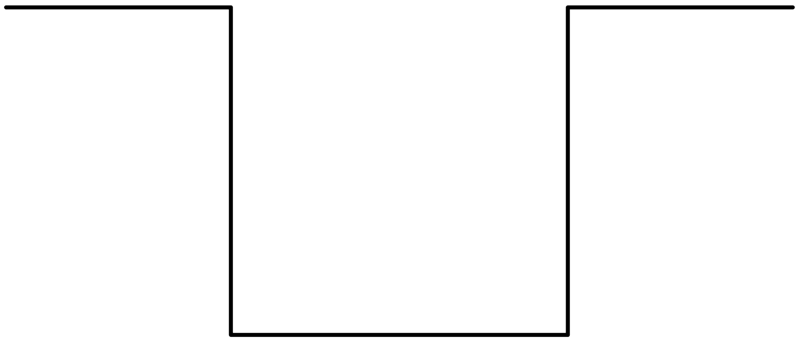
Coupled well

For zero barrier thickness

- we have a single well
  - of twice the thickness

This "finite well" problem can be solved relatively easily

- though the eigenenergy formula is not in closed form



Coupled well

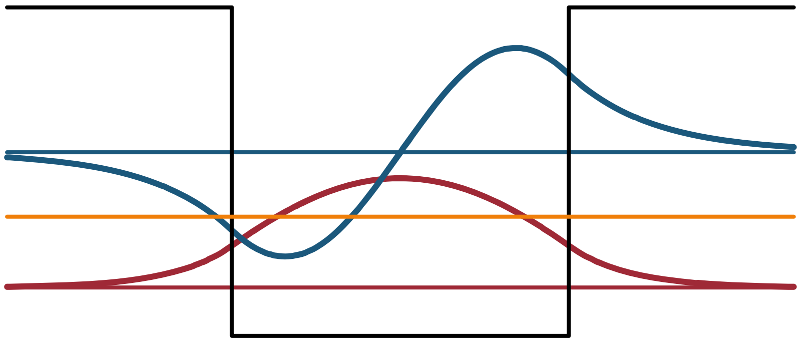
With finite barrier height

- we have "tunneling"
  - penetration into the barriers on either side

In this example

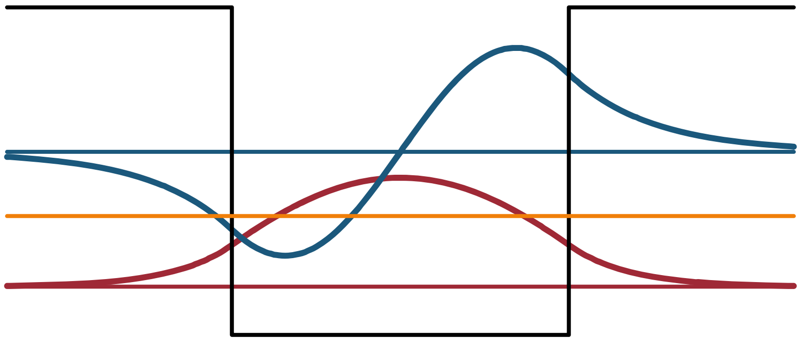
- we would find two energy levels "within" the well
  - a lower one
  - and a higher one

We add an orange line in the middle for future comparisons



Coupled well

With increasing barrier thickness



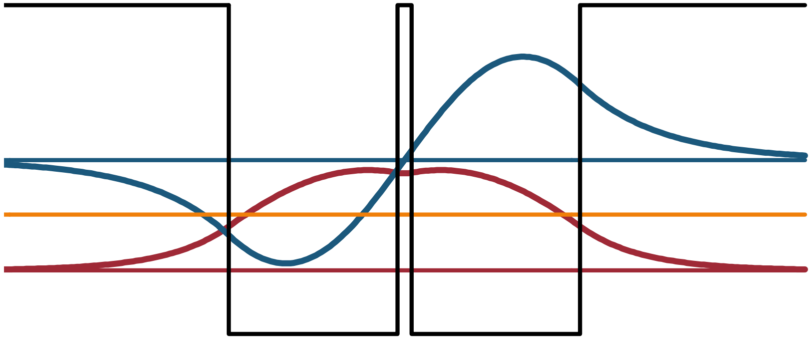
Coupled well

With increasing barrier thickness

- the energies get closer
  - and the problem transitions gradually towards
    - two weakly coupled wells

Note the symmetries of the wavefunctions are retained

- and the solutions are always for the coupled system



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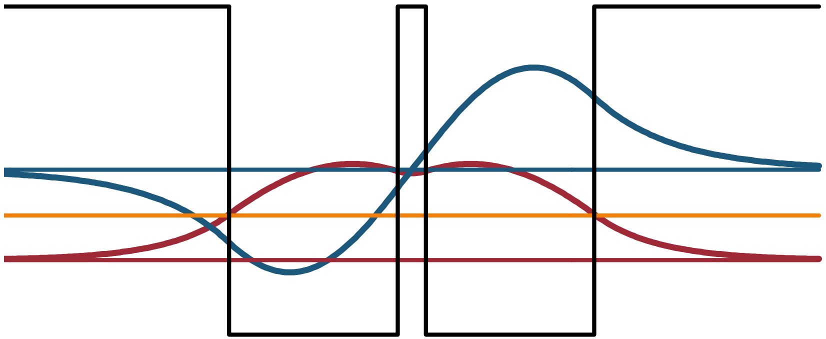

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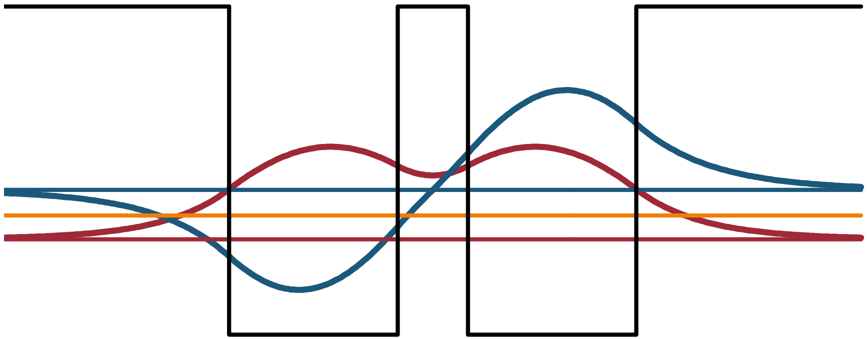

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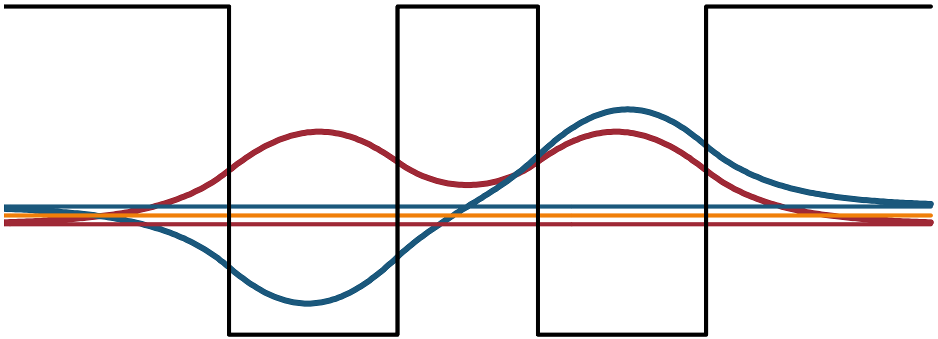

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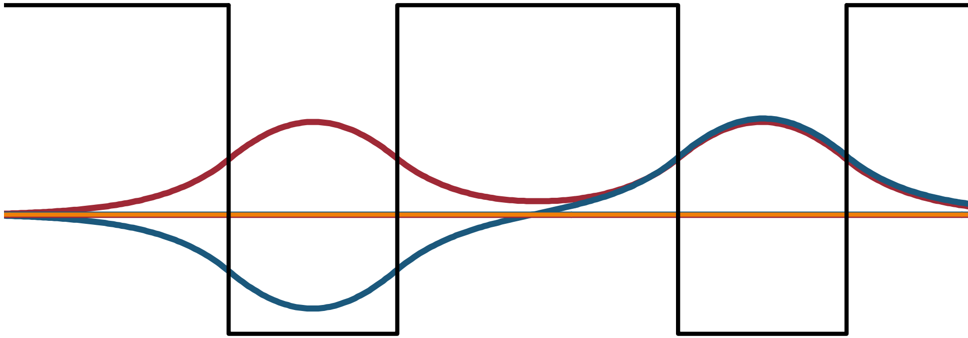
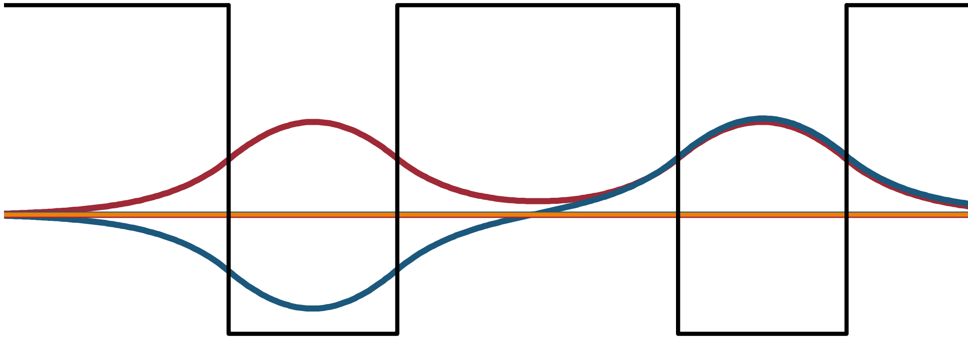


Coupled well

In the limit of a thick barrier

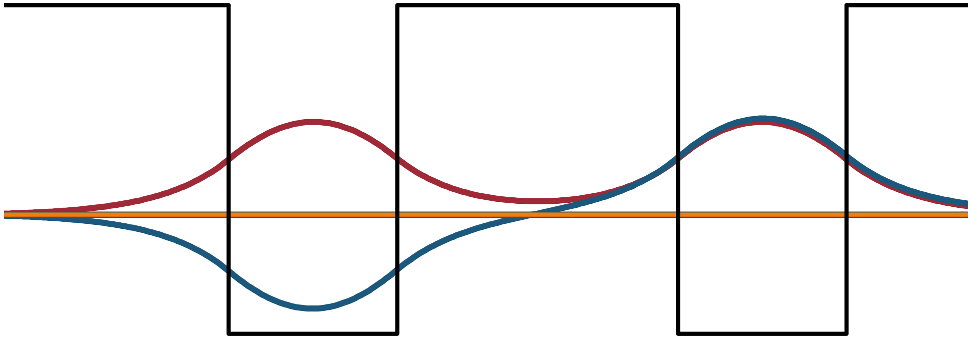
- one solution is the
  - "symmetric" combination of the "isolated well" solutions
- the other is the
  - "antisymmetric" one



Coupled well

Note that for thick barriers

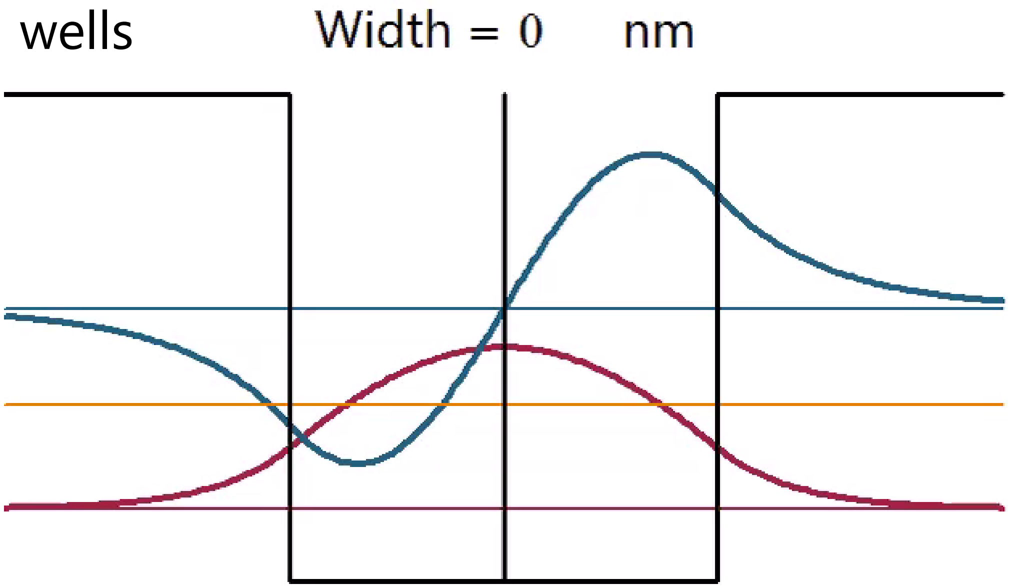
- both energies have
  - become very close to the orange line
    - which is the energy of the state in a single, isolated well



Coupled well solutions

1 eV barrier height

0.6 nm wide individual wells



0.362 eV

Bonding states

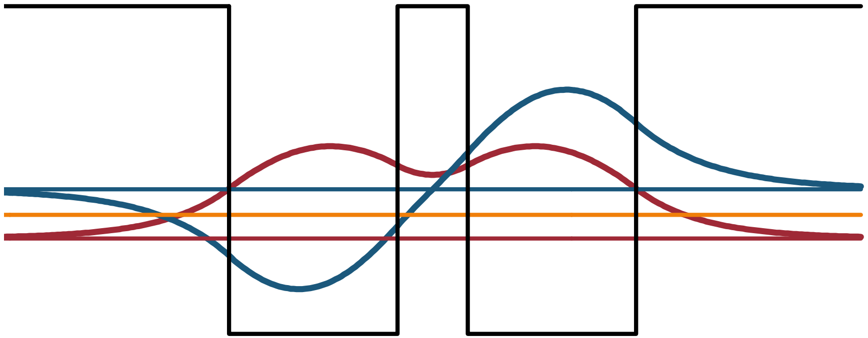
Note the energy of the lower state

- is below the energy of the "isolated well" solution

This is the essence of

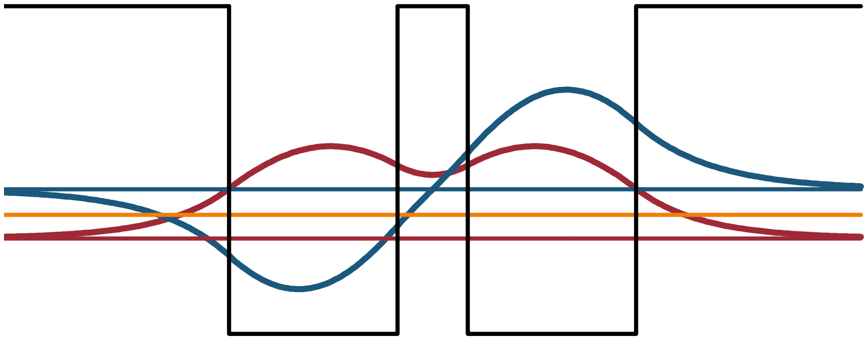
- covalent bonding of atoms in molecules

The energy is lower if they "share" an electron



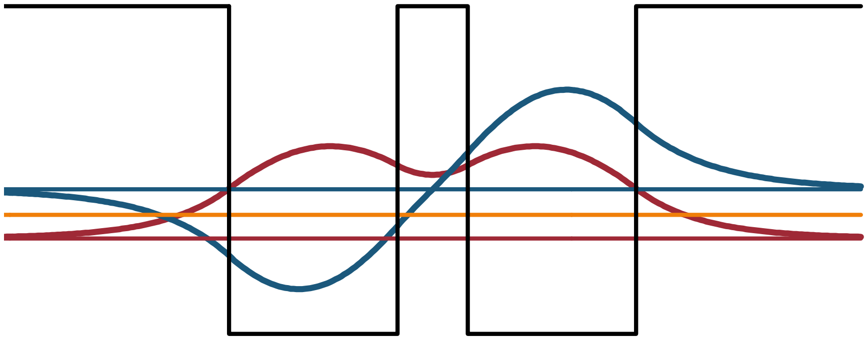
Bonding states

- In the lower, "bonding" state
  - the electron is more likely than before to be
    - in the region between the wells (or atoms)
- The energy is lower because
  - the wave function is less "curved"
    - giving a smaller "kinetic energy"



Bonding states

The higher energy
“antisymmetric” state
is sometimes called the
“antibonding” state
It has higher energy because
it is more strongly curved
giving larger “kinetic
energy”



Particles, atoms, and crystals 4

Crystals

Modern physics for engineers

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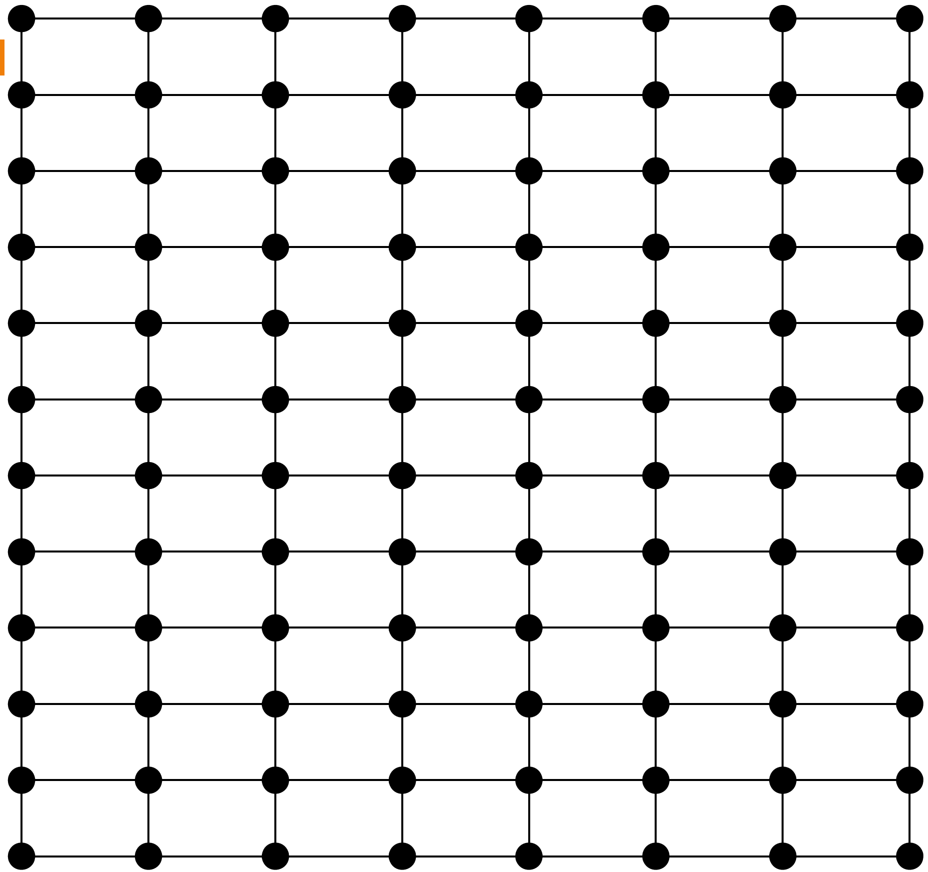
Crystal structures

A crystal

- is a material whose
  - measurable properties are periodic in space

A crystal structure

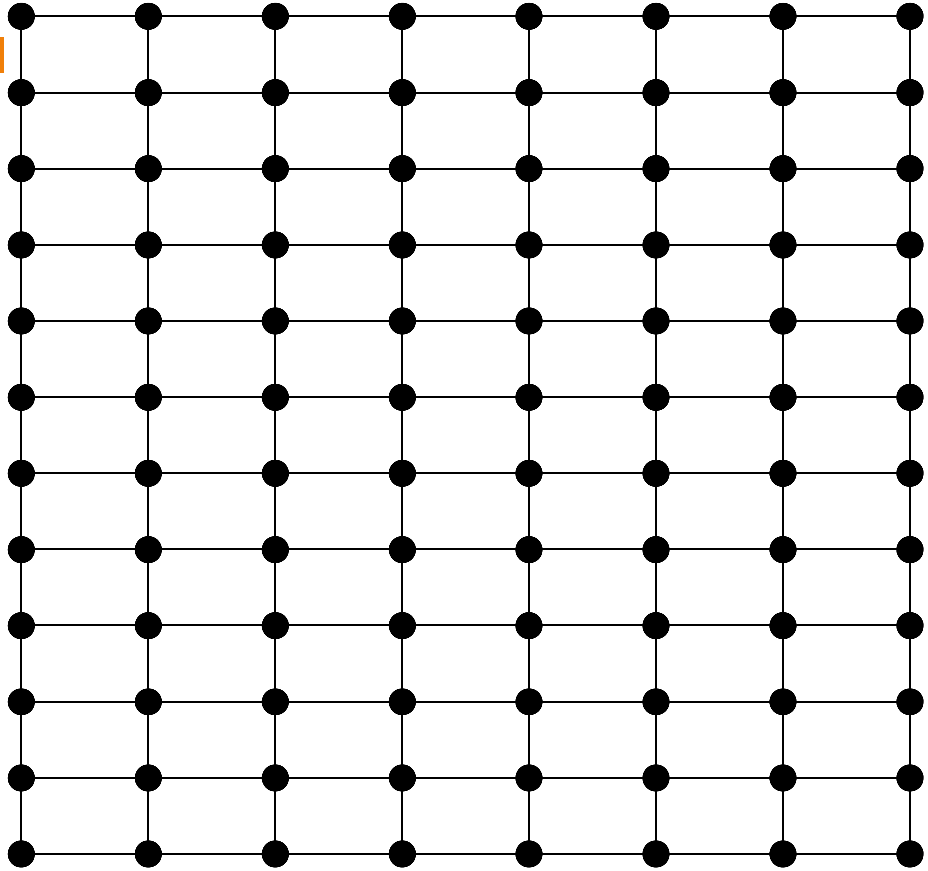
- is one that can fill all space
  - by the regular stacking of identical blocks or unit cells



Crystal structures

Crystal lattice

- If we put a mark on the same spot on the surface of each block
  - these spots would form a crystal lattice



Diamond and zinc-blende lattices

A large fraction of the semiconductor materials of practical interest

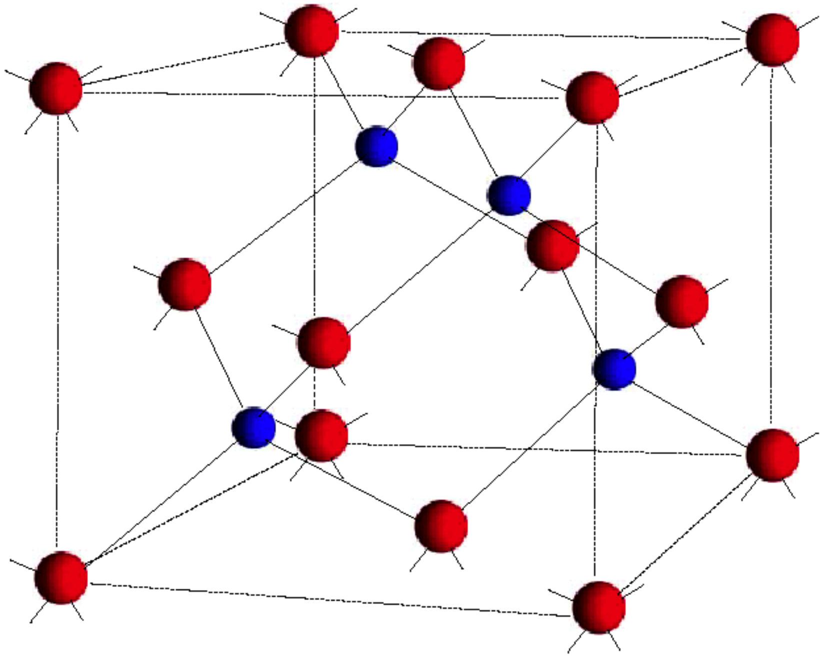
- such as silicon, germanium, and most of the III-V (e.g., GaAs) and II-VI (e.g., ZnSe) materials

have a specific form of cubic lattice

Diamond and zinc-blende lattices

In this form of lattice

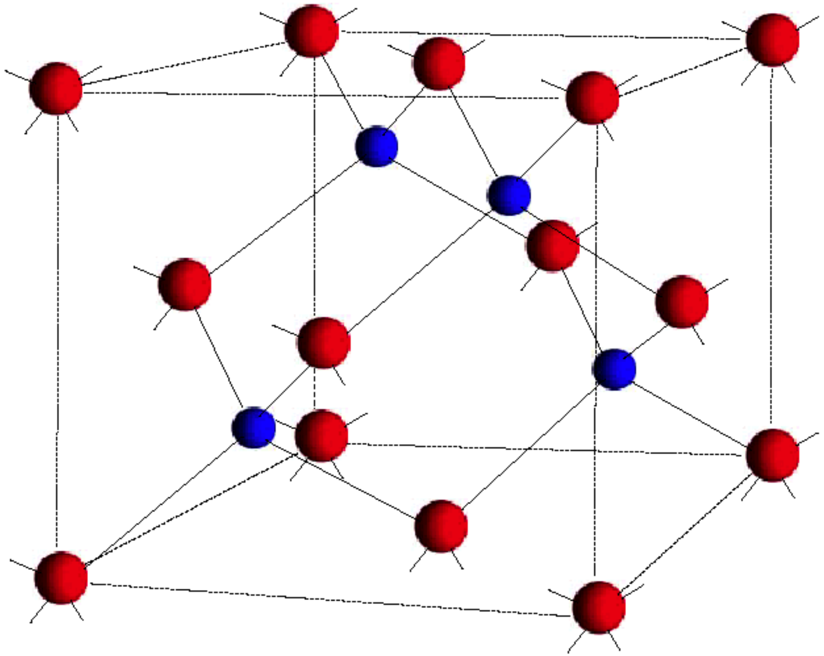
- each atom is bonded to four neighbors
  - Drawing a surface over the 4 “red” atoms round each “blue” atom
    - would give a regular
      - tetragon
        - with equal triangular faces



Diamond and zinc-blende lattices

Surprisingly

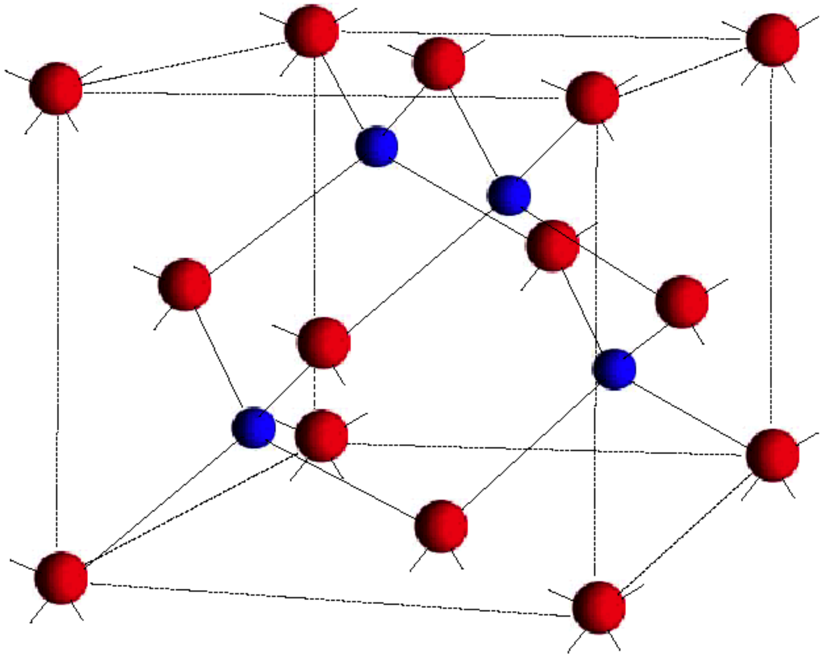
- this gives a kind of cubic lattice
  - a "face-centered cubic" lattice
    - with one "red" atom on each cube corner
      - and one in the middle of each cube face



Diamond and zinc-blende lattices

The actual physical lattice

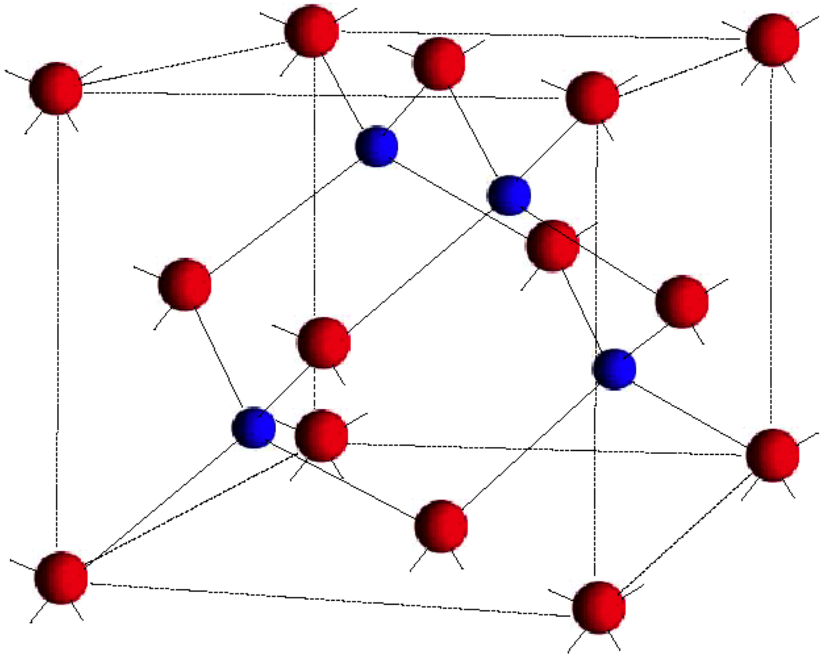
- has two interlocking face-centered cubic lattices
  - The “blue” atoms lie
    - on another similar “face-centered cubic” lattice
      - shifted over by one bond



Diamond and zinc-blende lattices

"Zinc-blende" is the crystal structure for

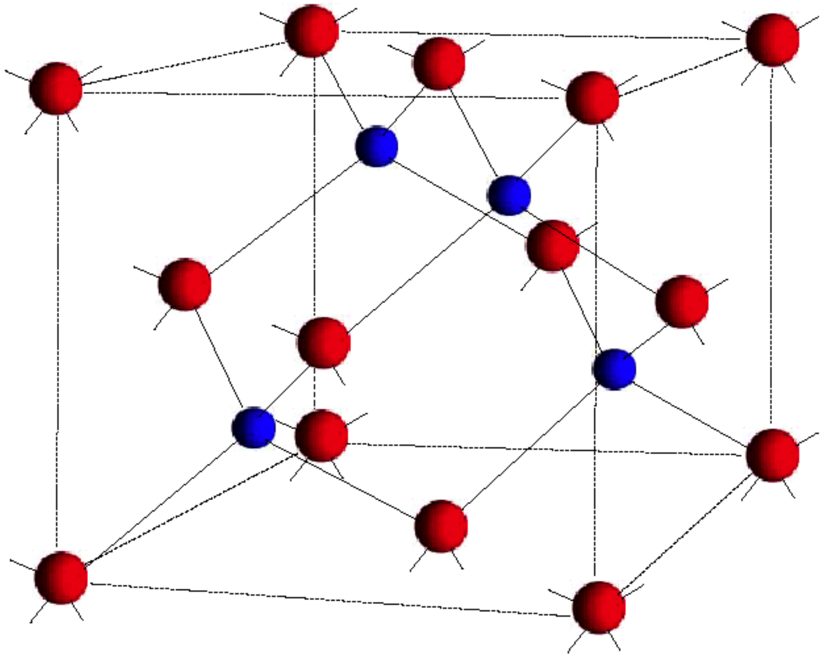
- most III-V and II-VI materials
  - The group III (or II) atoms lie on one such face-centered cubic lattice
  - and the group V (or VI) lie on the interlocking face-centered cubic lattice



Diamond and zinc-blende lattices

"Diamond" is the lattice for
- some group IV materials
  - e.g., silicon, germanium
  - some forms of carbon (diamond itself) and tin

Both interlocking lattices
- have the same kinds of atoms on them



Other important semiconductor lattices

- Hexagonal
  - as in the graphite form of carbon
    - also graphene
      - a single sheet of hexagonal carbon atoms
    - and the basis of carbon nanotubes
      - rolled up sheets of hexagonal carbon atoms
- Wurtzite
  - a form of hexagonal lattice with two atoms per lattice point

Alloy semiconductors

Alloy semiconductors

Alloy semiconductor materials

made from mixtures of elements

for example

of Group III elements on the Group III sublattice

and/or

of Group V elements on the Group V sublattice

are important especially for optoelectronic devices

Alloy semiconductors

Though the random distribution of elements

- means these alloys are technically not crystals
  - in practice we treat them as crystals
    - with averaged properties of the perfect crystals
      - The perfect crystals would be "binary"
        - having only two component elements

III-V semiconductor alloys

III-V semiconductor alloys

- Alloy semiconductor materials include
  - ternary (three component) alloys, e.g.,
    - indium gallium arsenide
      - where the Group III face-centered cubic sublattice has
        - a random distribution of indium and gallium atoms
    - aluminum gallium arsenide

III-V semiconductor alloys

- quaternary (four component) alloys, e.g.,
  - indium gallium arsenide phosphide
  - indium gallium aluminum arsenide
- These alloys give flexibility in design of material properties
  - allowing, e.g., choice of the wavelength of light emitted

Non-crystalline materials

Crystalline and non-crystalline materials

- Usually, we make semiconductors crystalline because
  - we need the best controlled performance from them
- Other materials also used in making devices, such as
  - metals for conductors and
  - oxides for insulators
    - often do not need precise crystalline forms to operate successfully

Crystalline and non-crystalline materials

- Non-crystalline materials can often be made by simple techniques
  - such as evaporation onto the surface
- Growth of crystals usually requires
  - carefully controlled temperatures
  - growth on some substrate or seed that itself is crystalline
    - with the same separation between the atoms

Crystalline and non-crystalline materials

- Such seeded growth is called "epitaxial"
  - meaning that the growing surface
    - takes on the order of what lies beneath it
      - "epi" meaning surface (as in "epidermis")
        - and the "tax.." as in "taxonomy"
          - meaning an ordering

Particles, atoms, and crystals 4

Emergence of bands

Modern physics for engineers

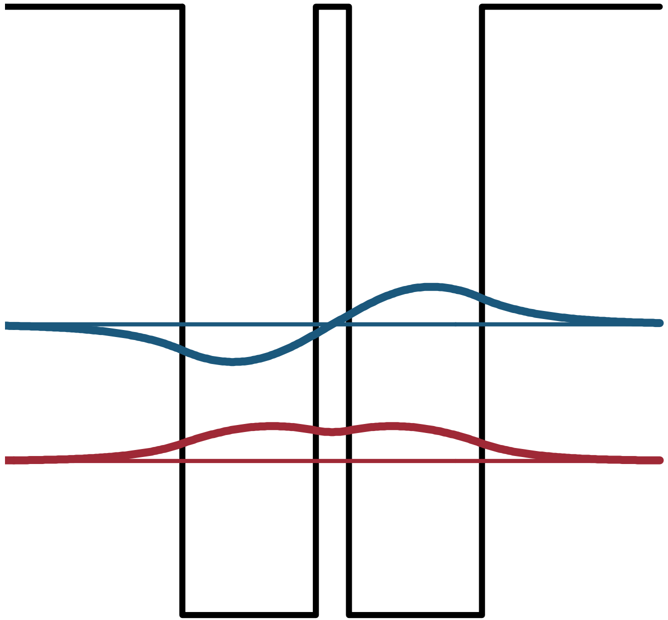
David Miller

Coupling multiple identical systems

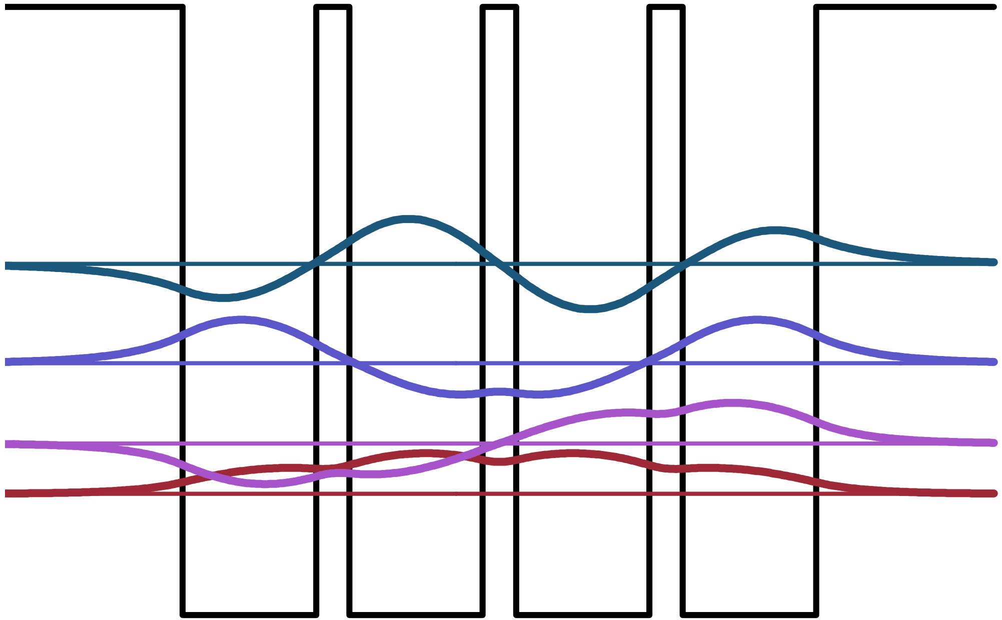
What happens when we bring multiple "atoms" closer together?

- Answer:
  - For N identical systems
    - each original level
      - will split into N levels in the coupled system

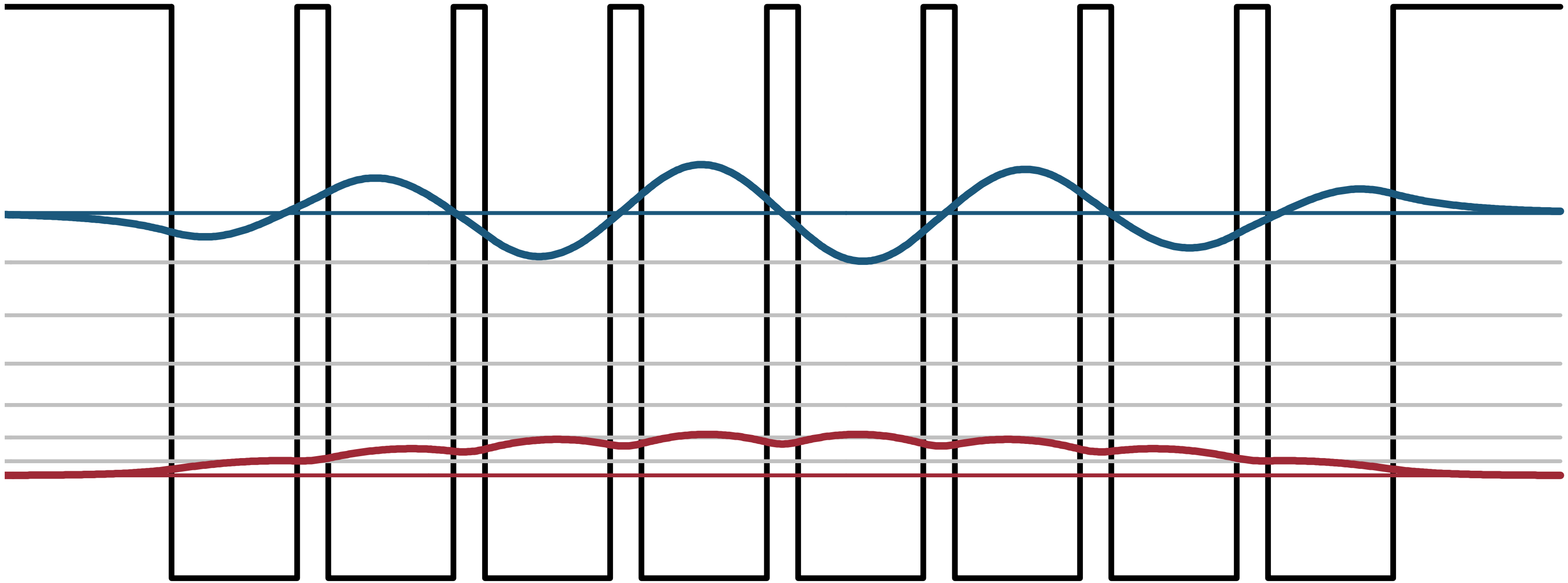
Coupling multiple identical systems



Coupling multiple identical systems



Coupling multiple identical systems



Bands of states

As we increase the number of coupled wells or "atoms"

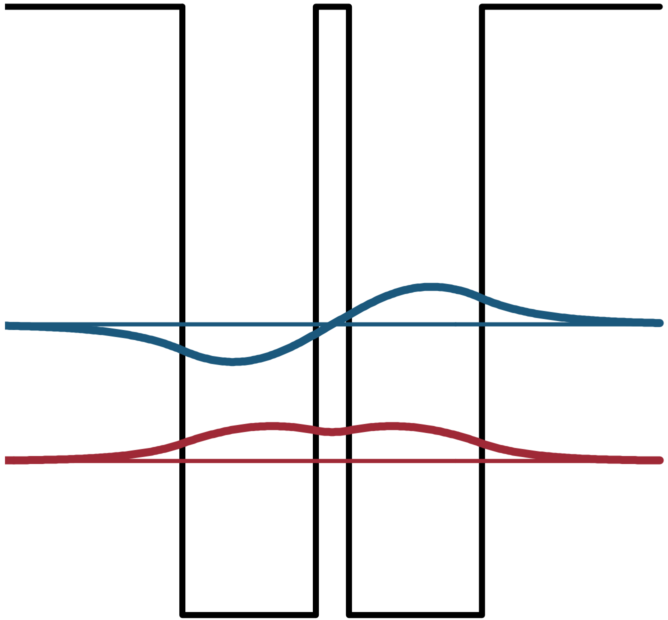
- we call the resulting groups of coupled states "bands"

Bands of states

Notice that, as we increase the number of coupled wells

- the separation between
  - the lowest energy
  - and highest energy coupled states
- increases
  - but it starts to "saturate"
    - tending towards a limit as we increase the number of wells

Coupling multiple identical systems



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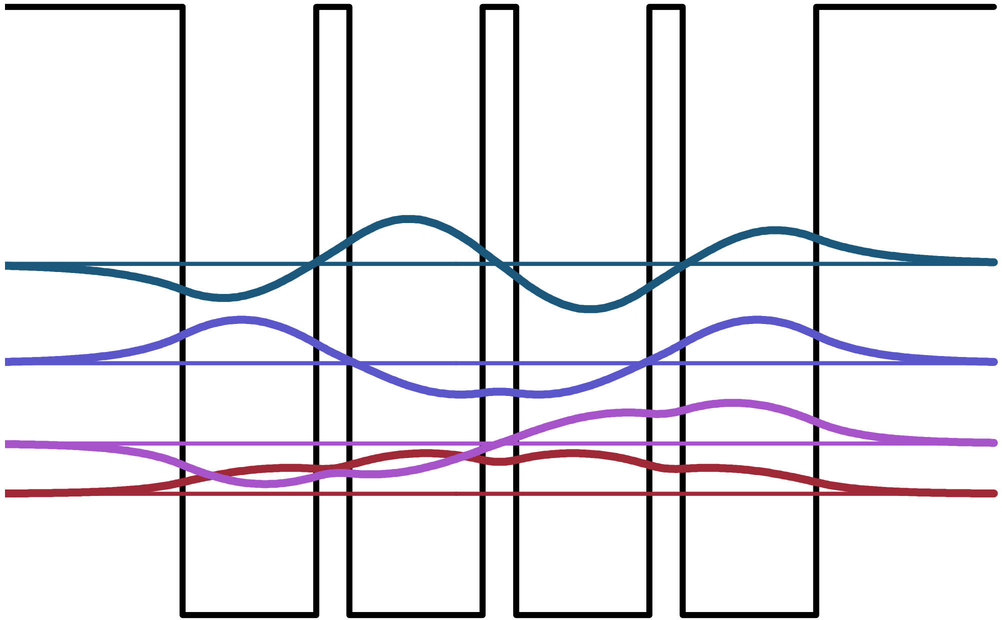

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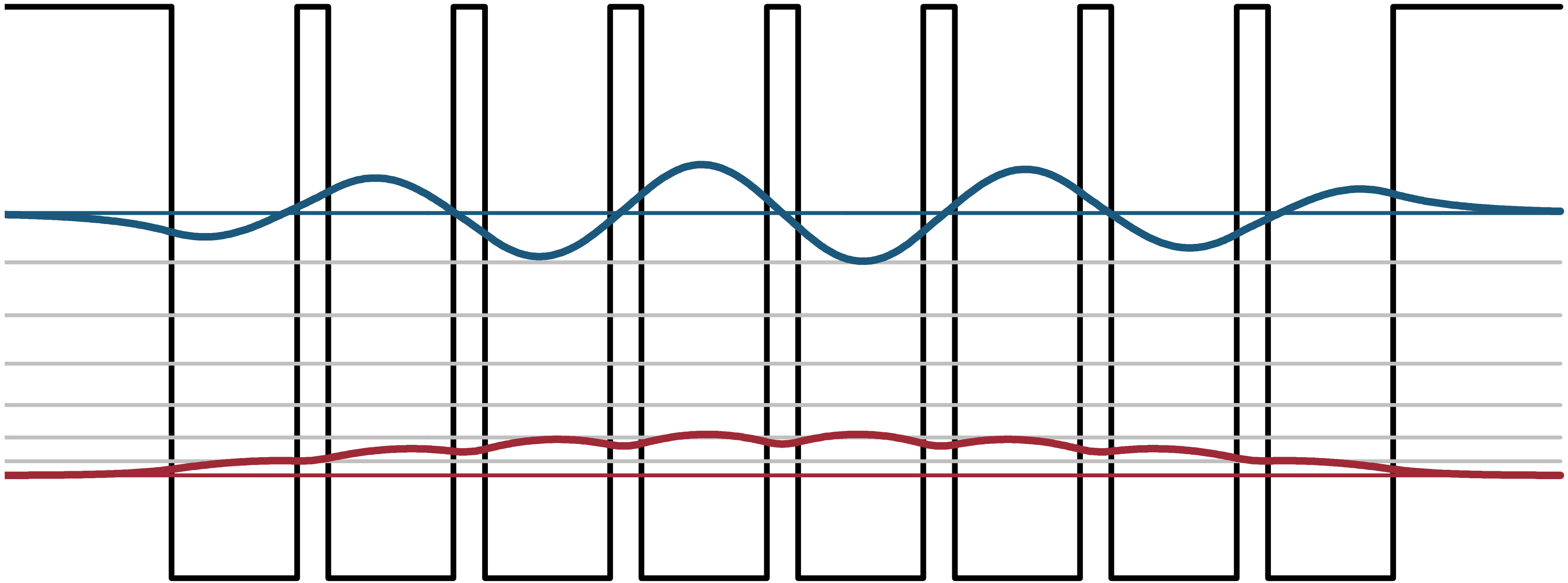
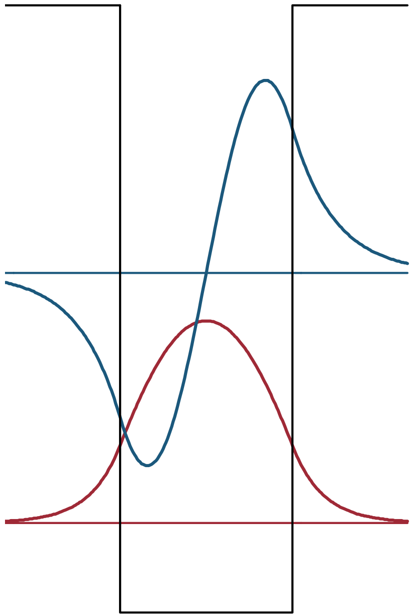


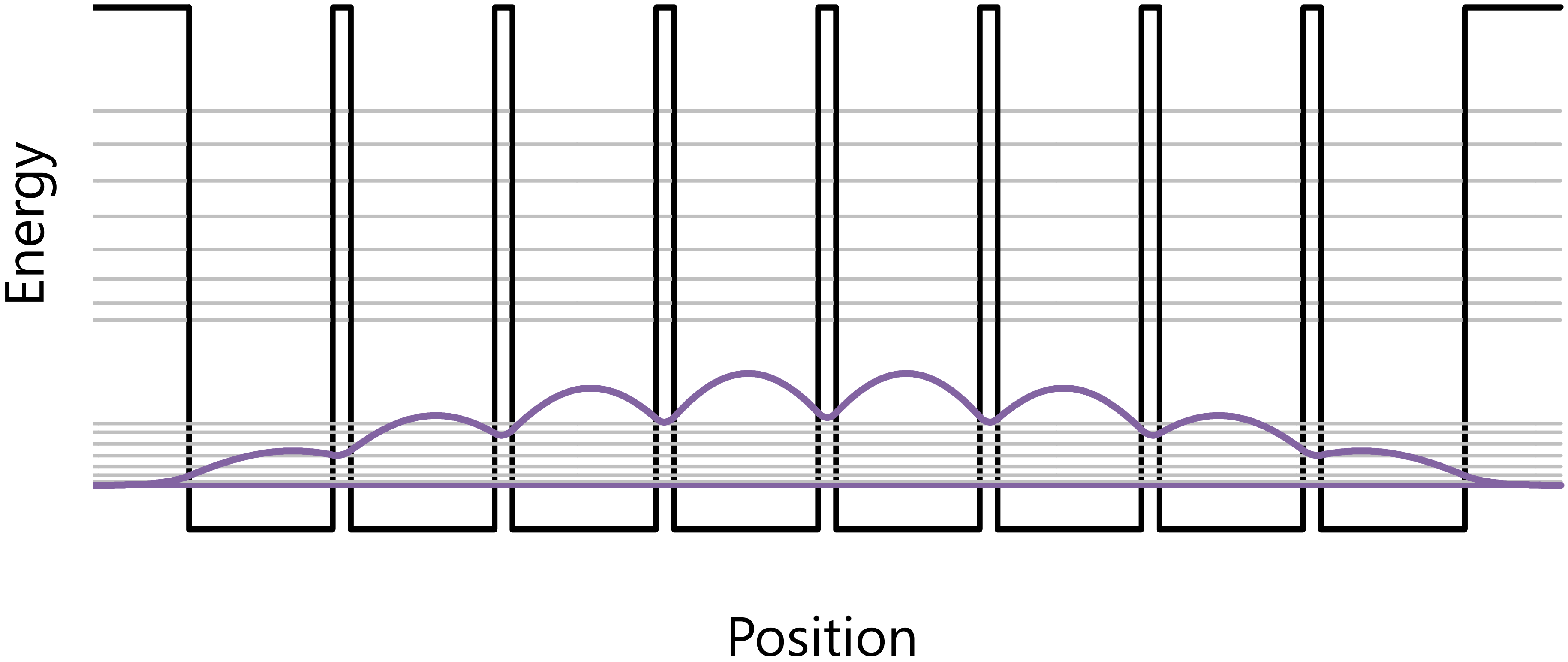
Multiple bands



For a wider well

- we could have two levels
  - each of which could split into bands

States for 8 coupled wells



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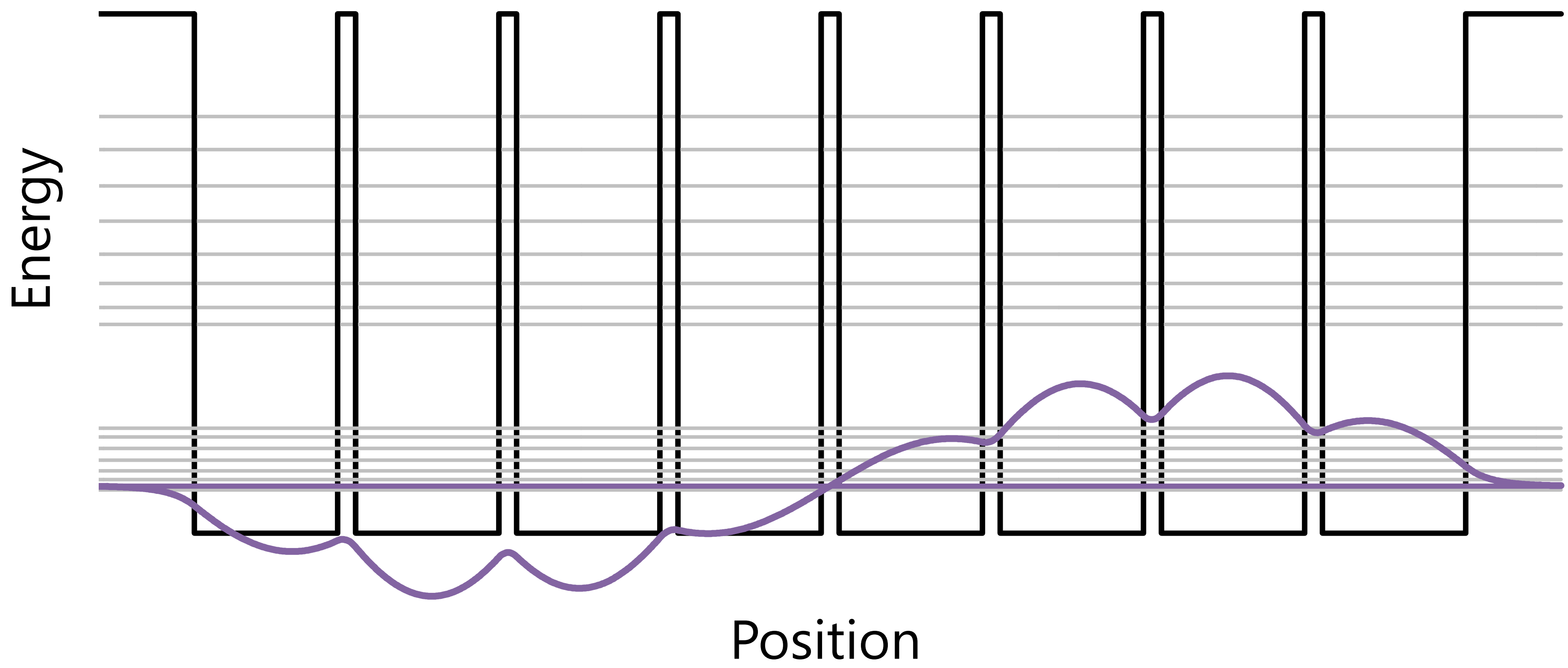

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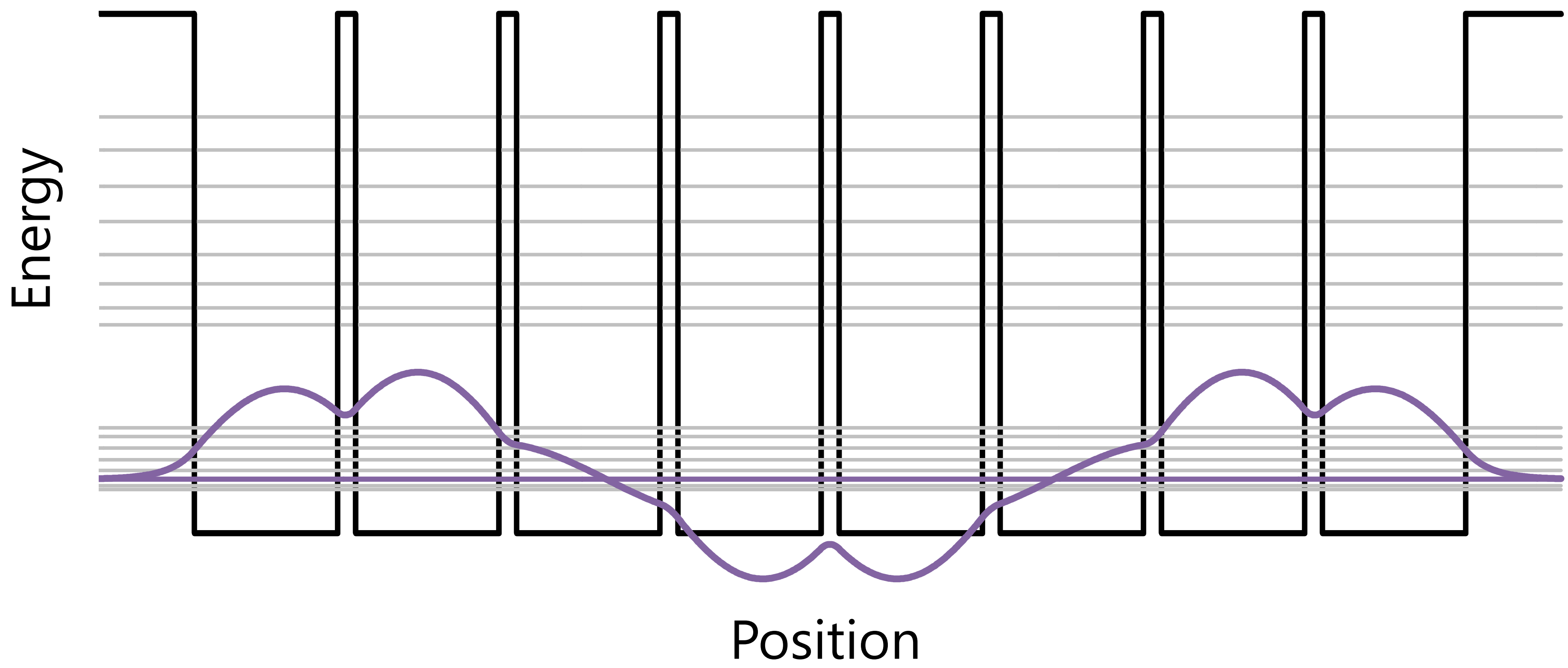

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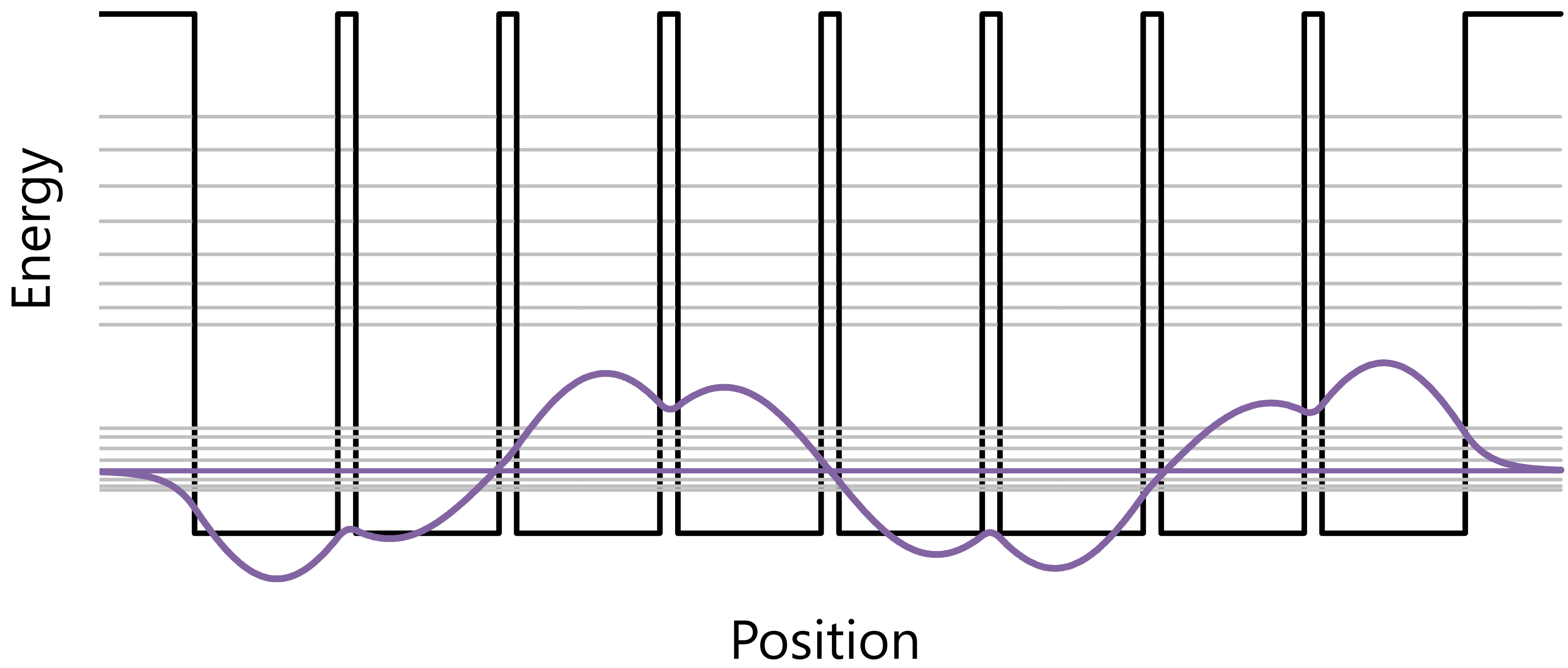

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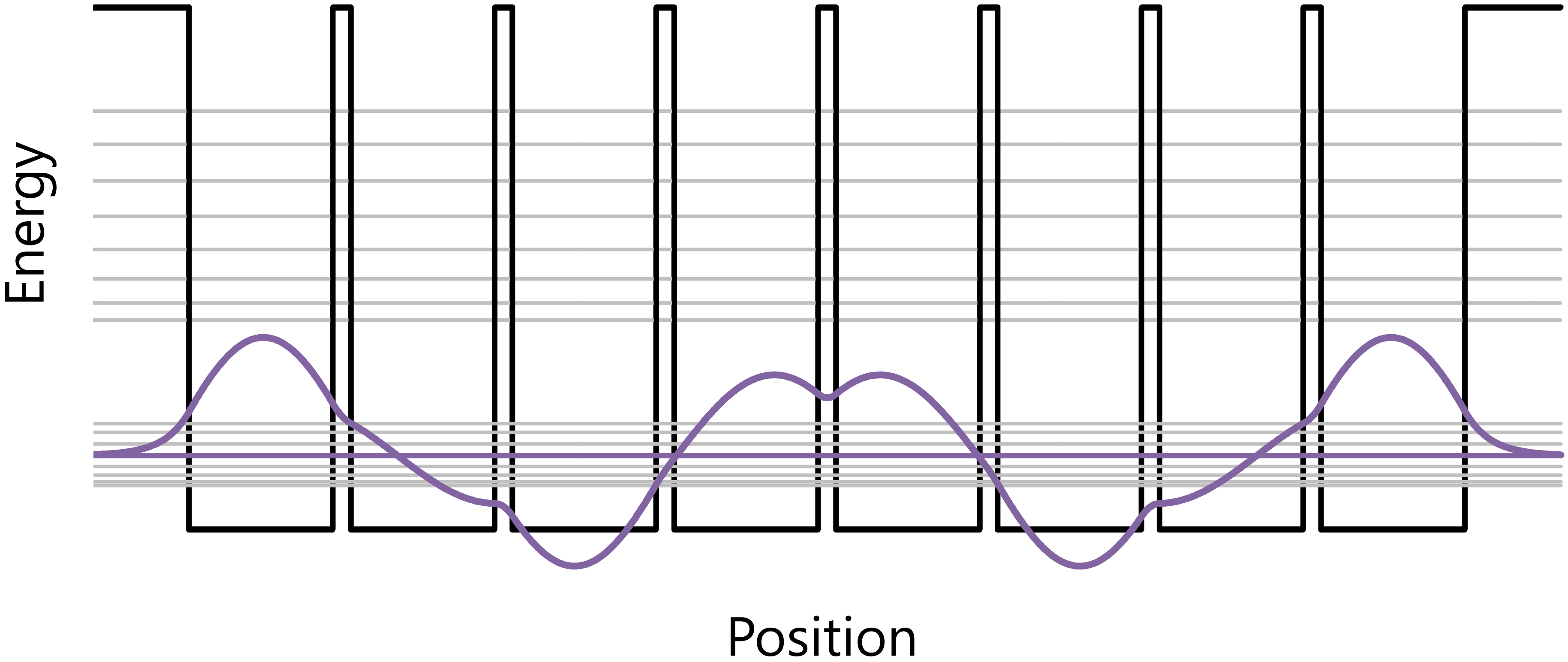

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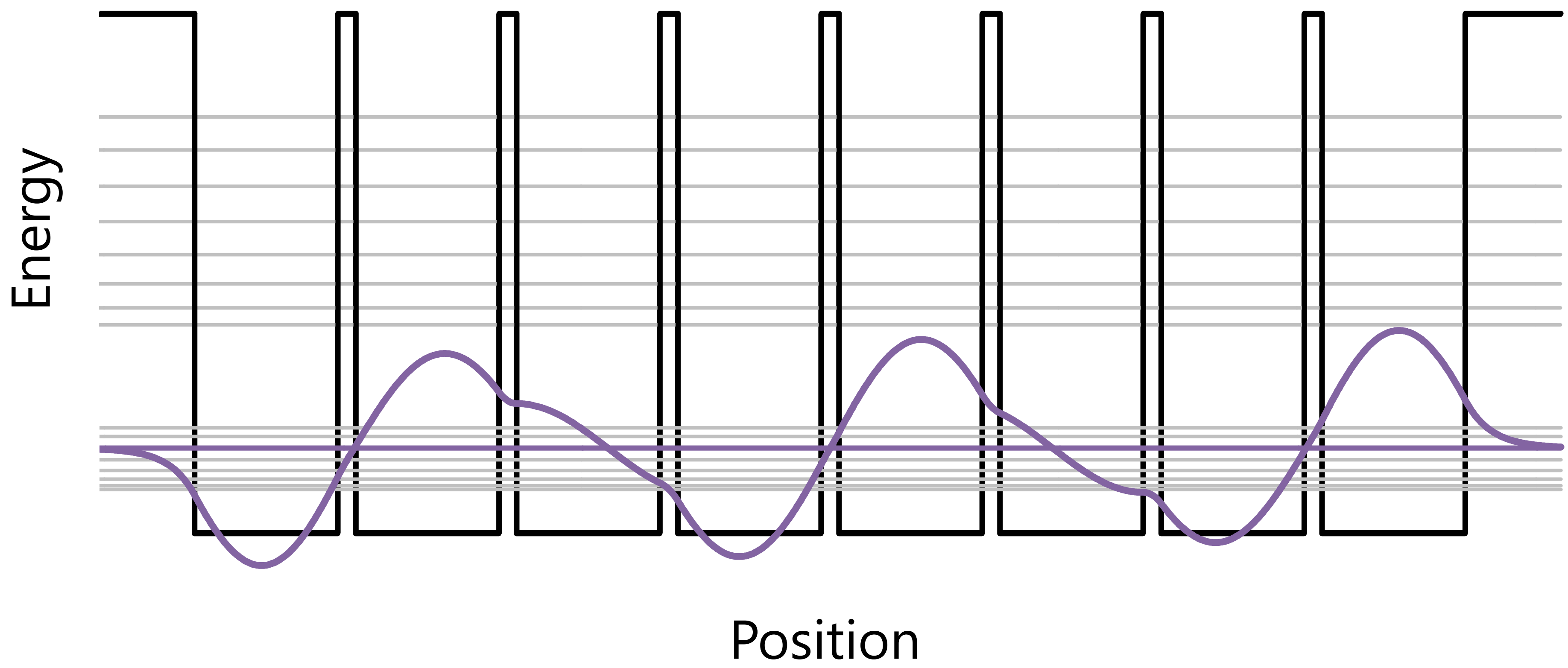

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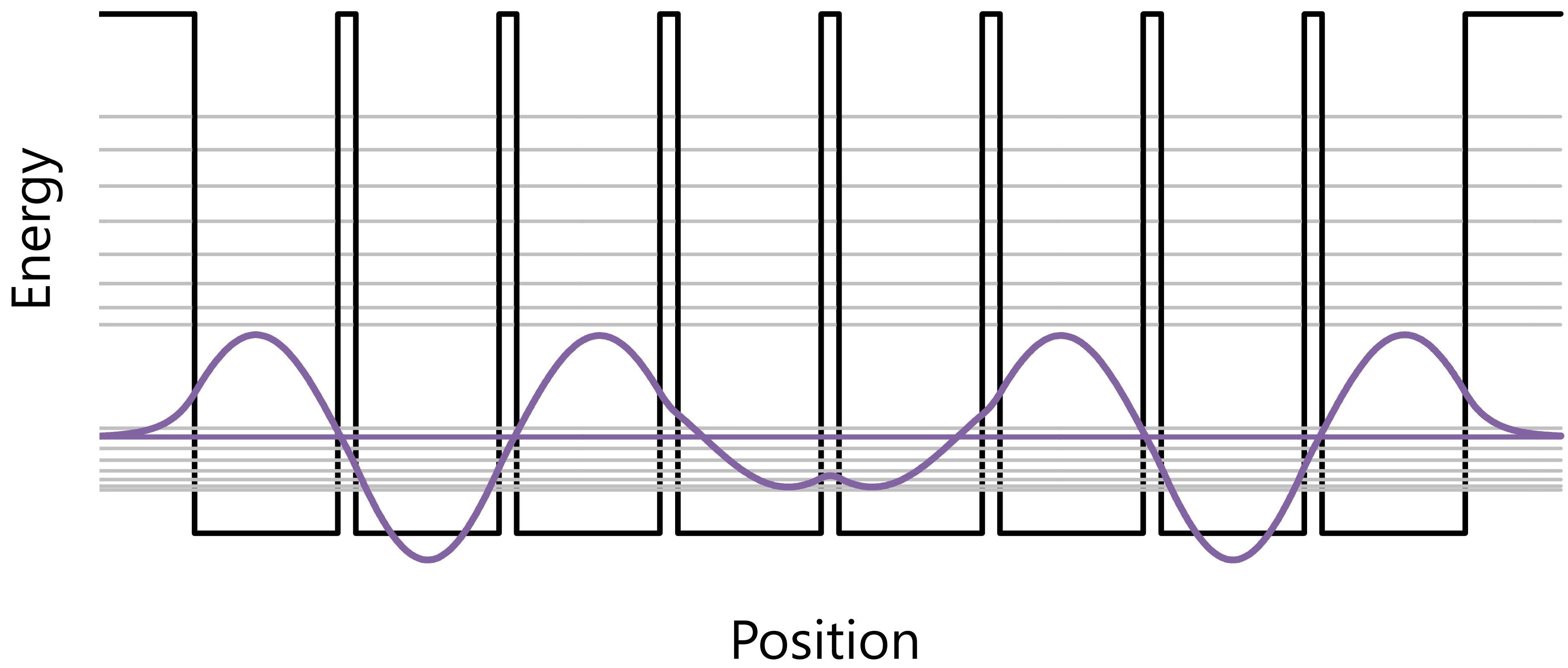

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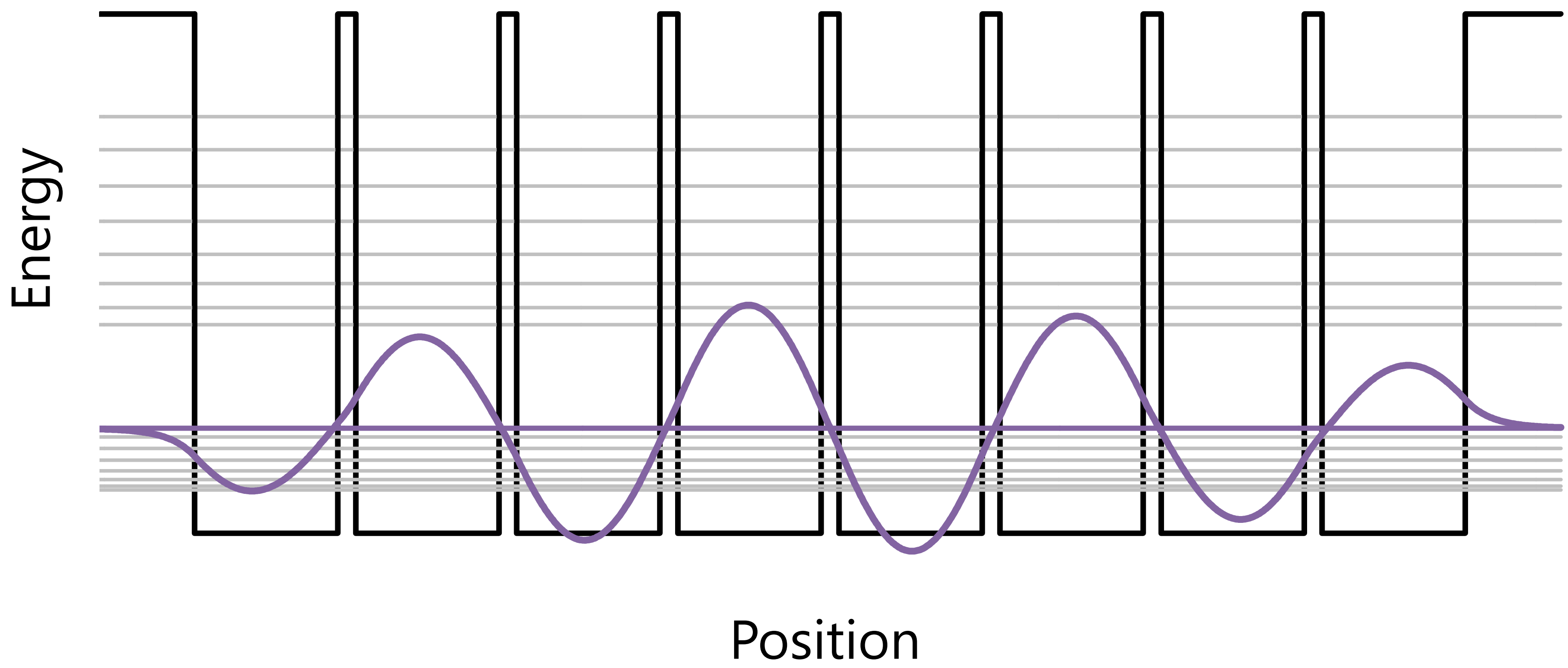


Wavefunctions in "bands"

These wavefunctions are a product of

- (i) a "unit cell" function that is essentially the "isolated well" function, and
- (ii) an overall standing-wave "envelope" function

For the lowest state in this band

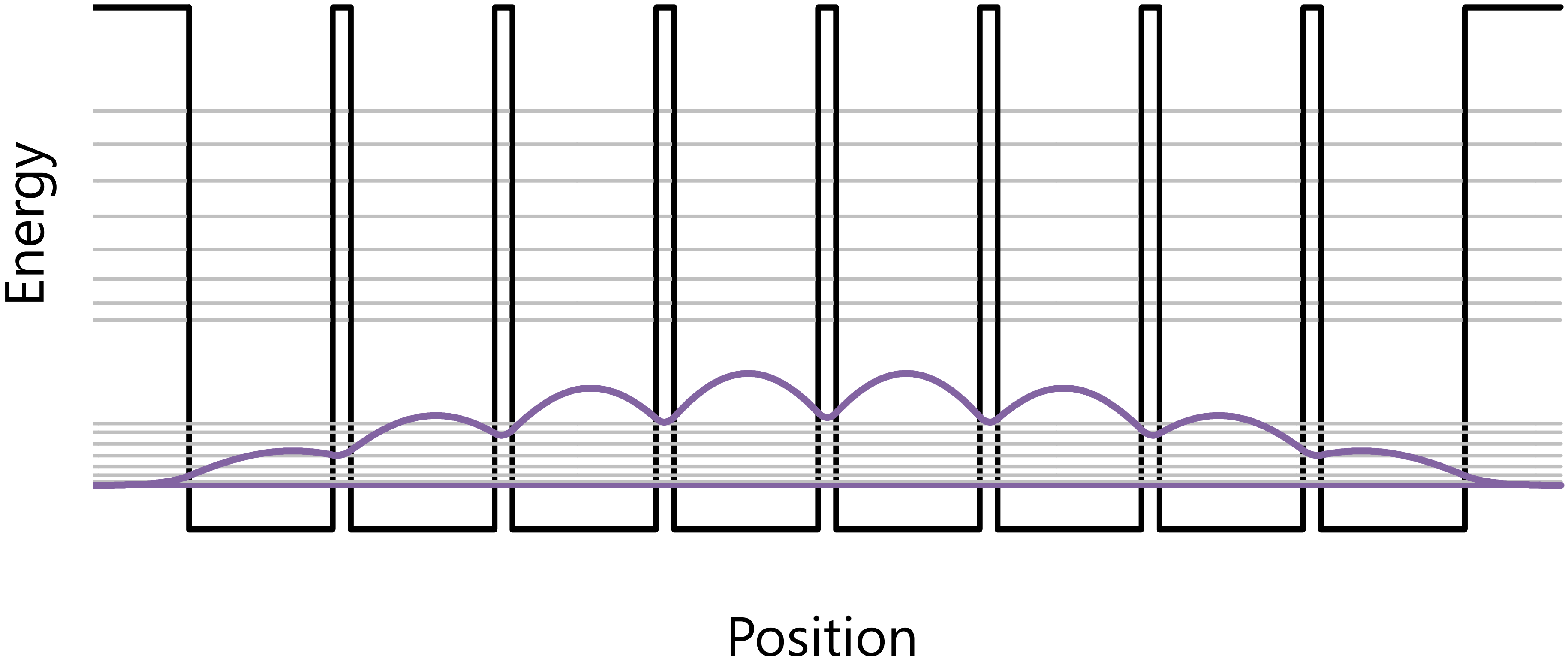
- we can see an overall standing-wave "envelope" pattern corresponding to one half-wave of a sine wave
  - just like a wave on a string or a particle in a box that is "modulated" by one "bump" per well

Wavefunctions in “bands”

For the highest state in this band
- the wavefunction is changing sign between adjacent wells
  - because the isolated-well function is multiplied by an envelope
    - that has 4 full waves (or 8 half-waves) between the “walls”

For the other levels
- the “envelope” function for each successive higher energy state
  - has one more half-wave in it

States for 8 coupled wells



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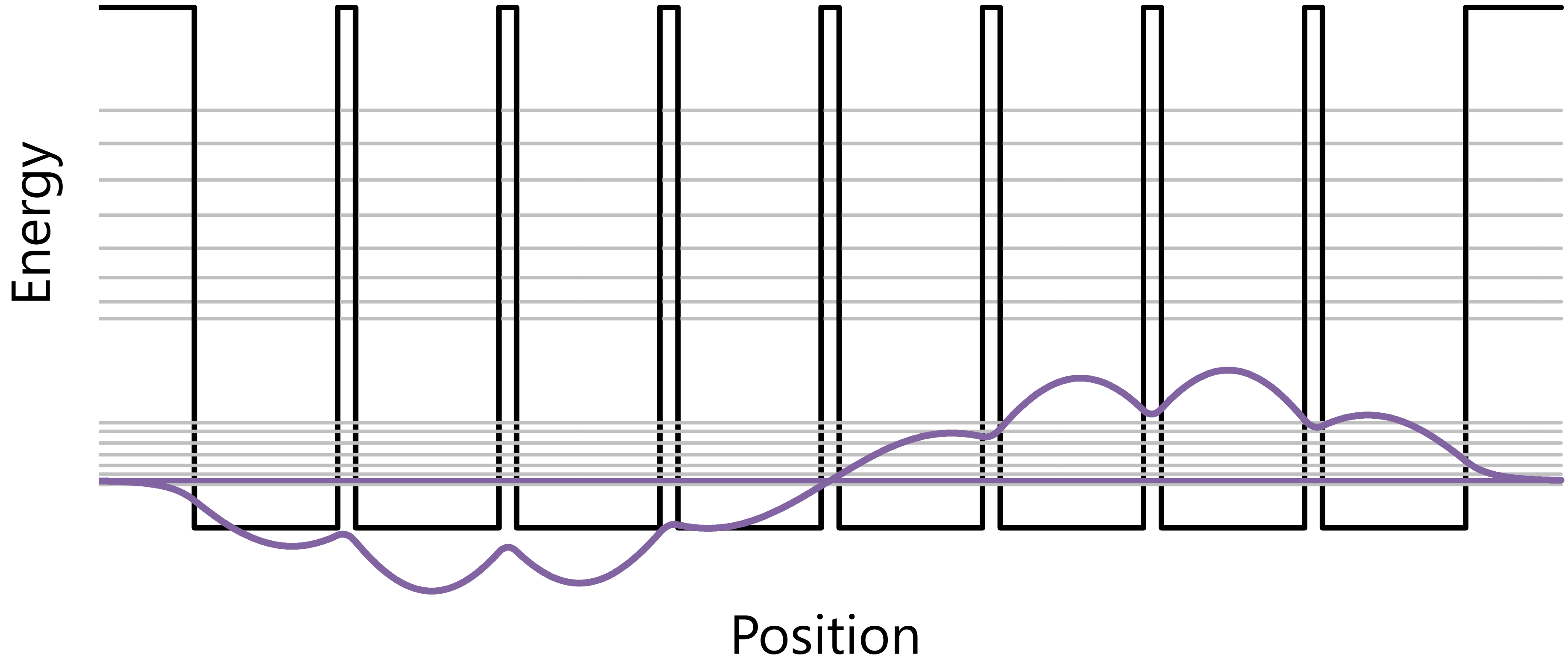

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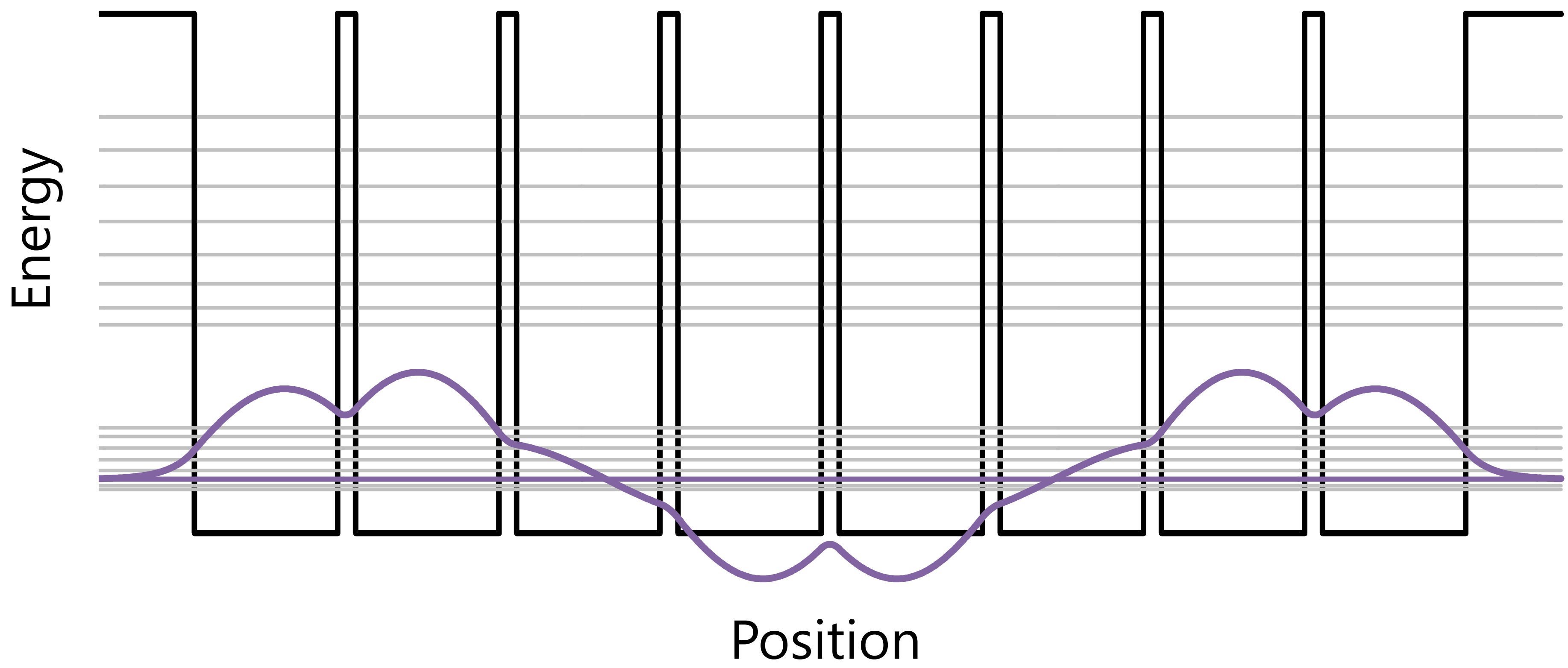

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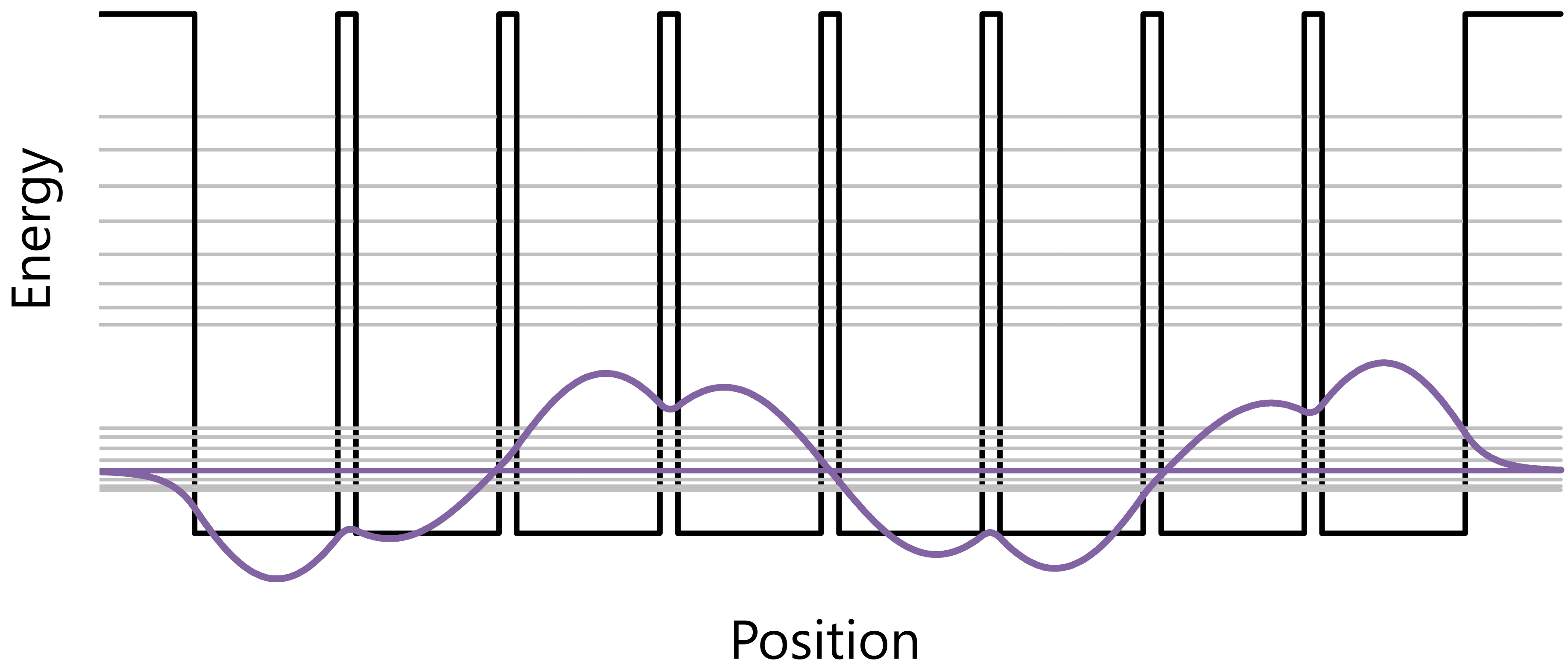

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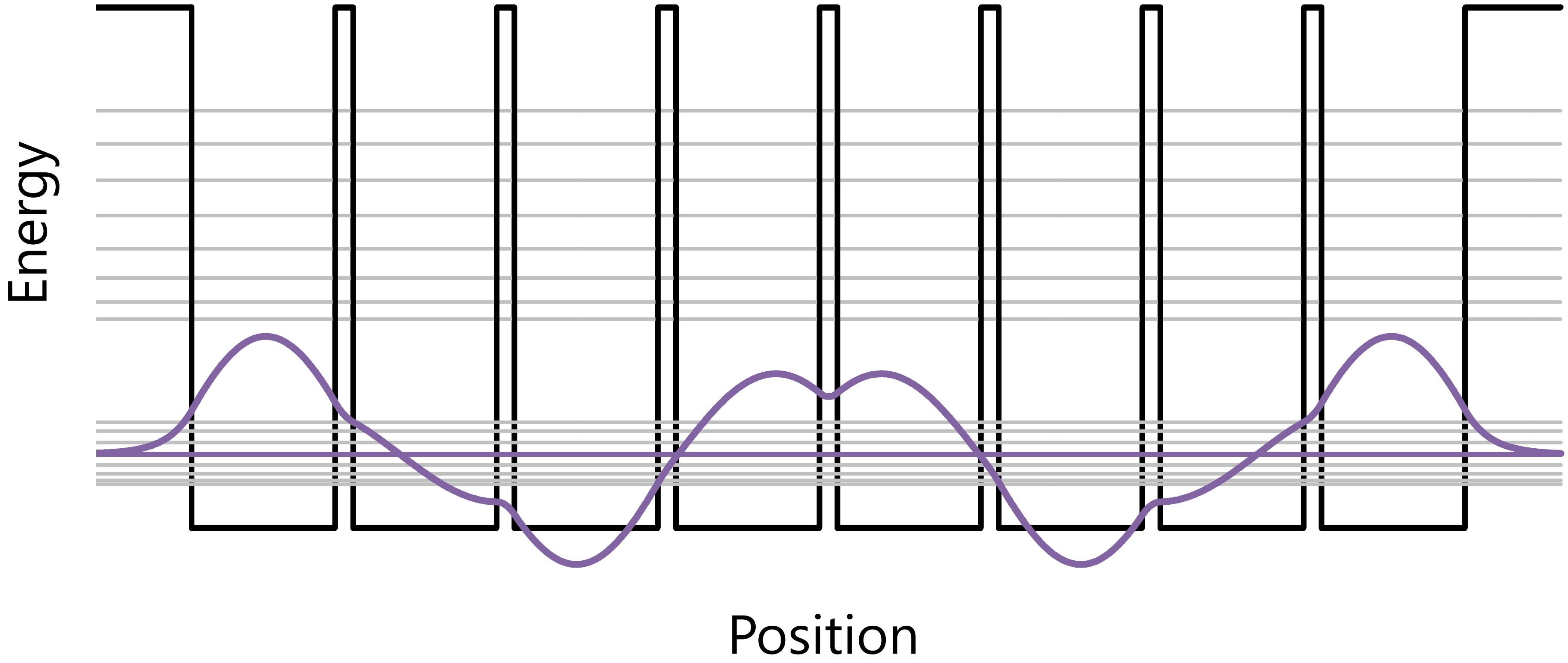

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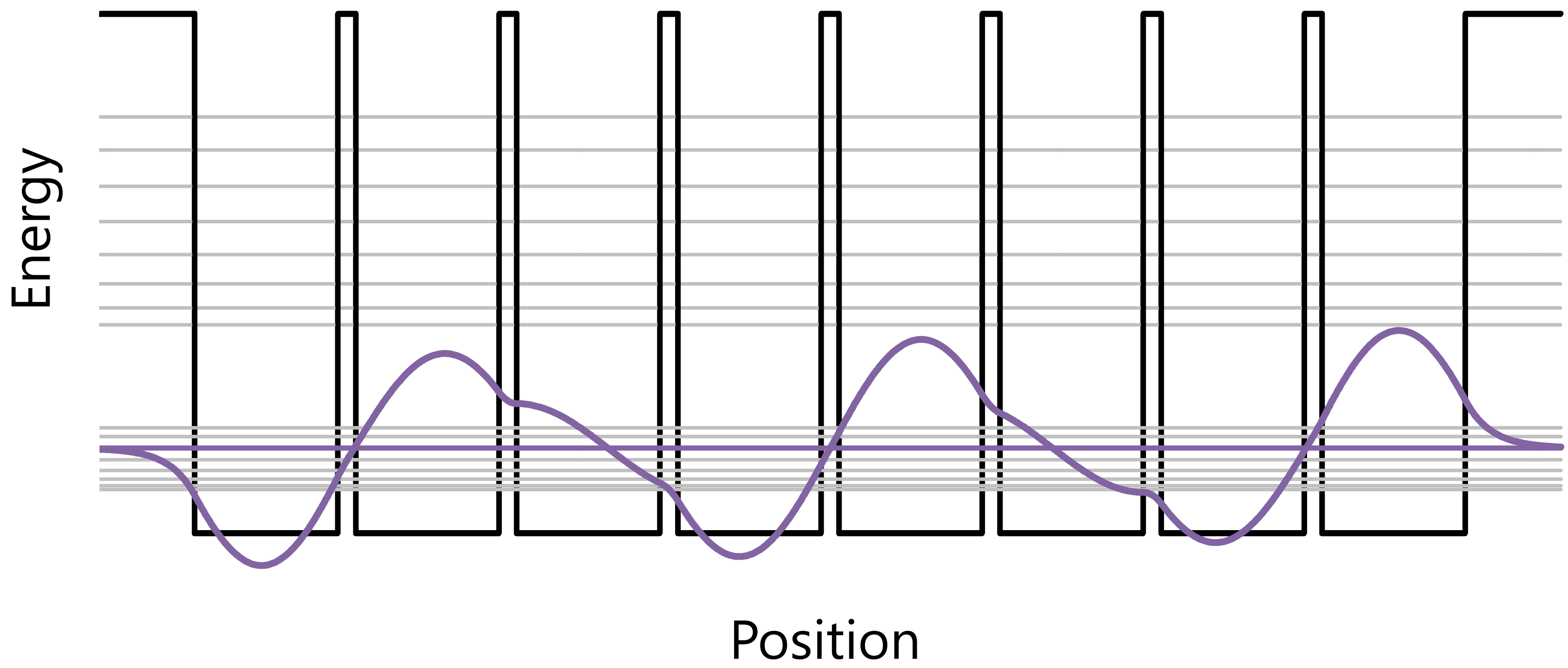

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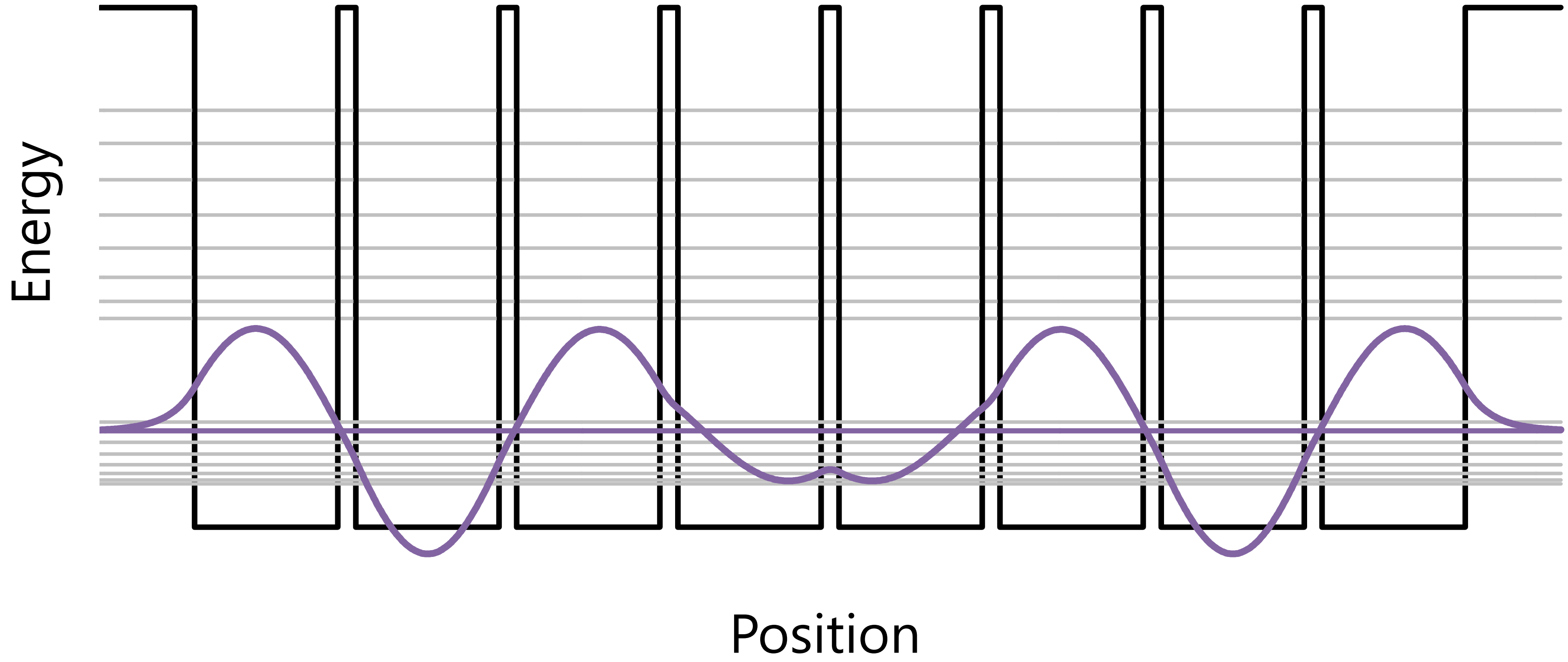

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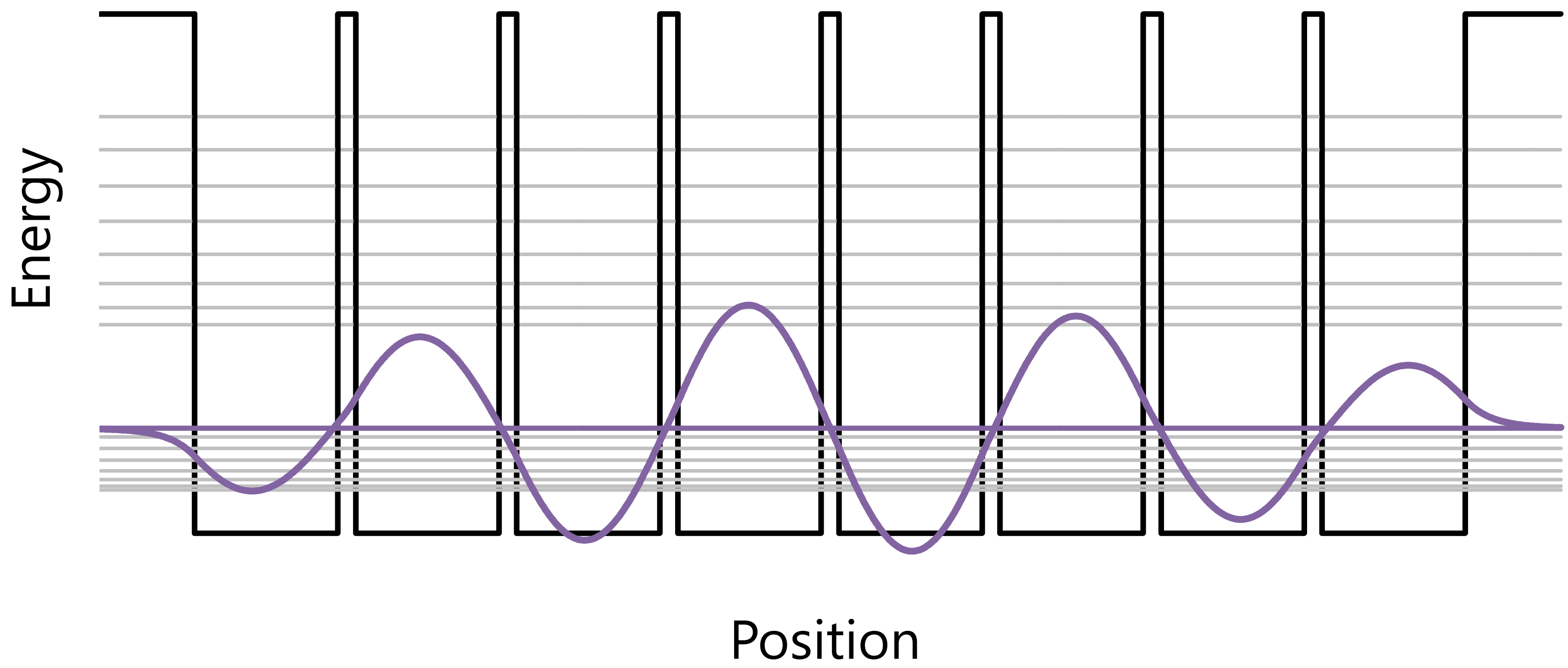
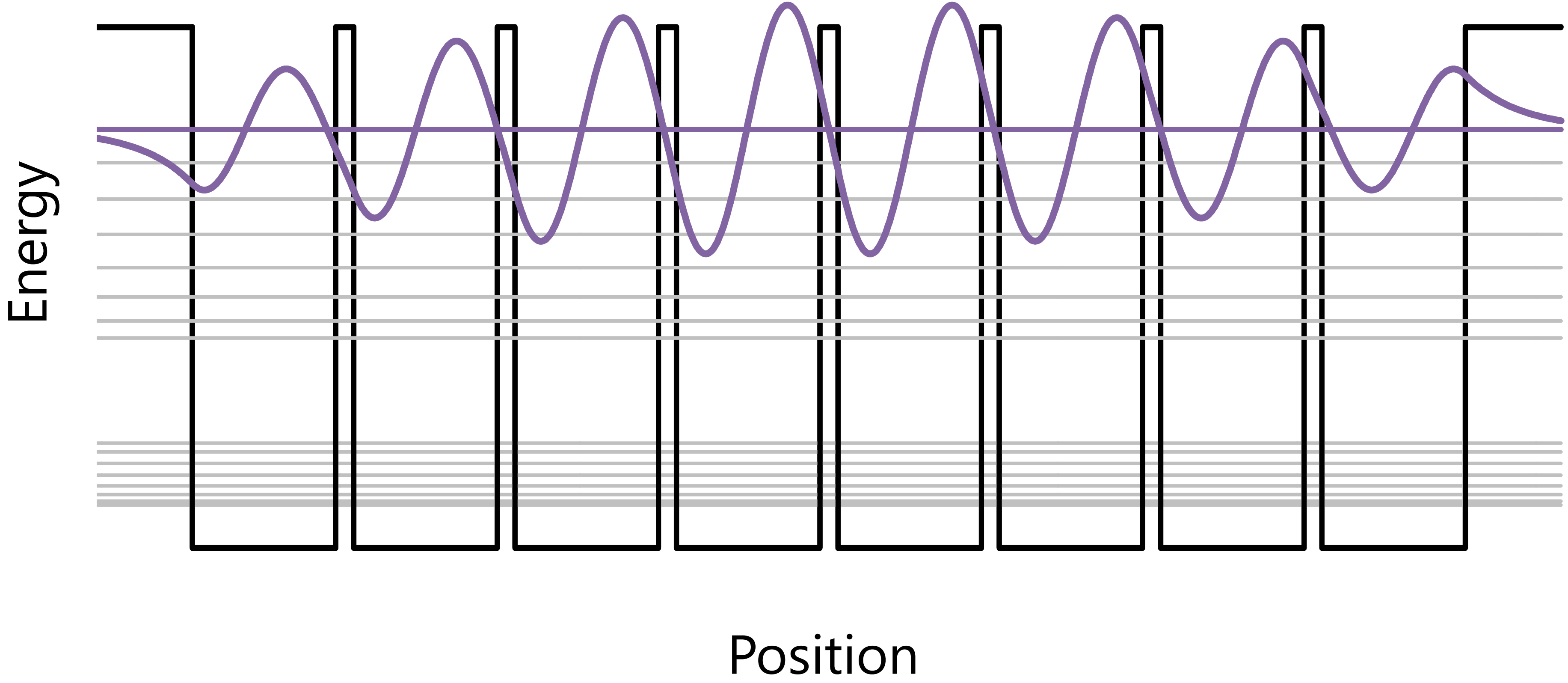


Wavefunctions in "bands"

For the next band we see similar behavior except

- the "unit cell" wavefunction is the second state in the isolated well
  - with a zero in the middle
- the energy ordering of the "envelope" functions is inverted
  - The "single half wave" envelope function is for the highest energy state
    - Note the most highly "curved" wavefunction
      - still has the highest energy

States for 8 coupled wells



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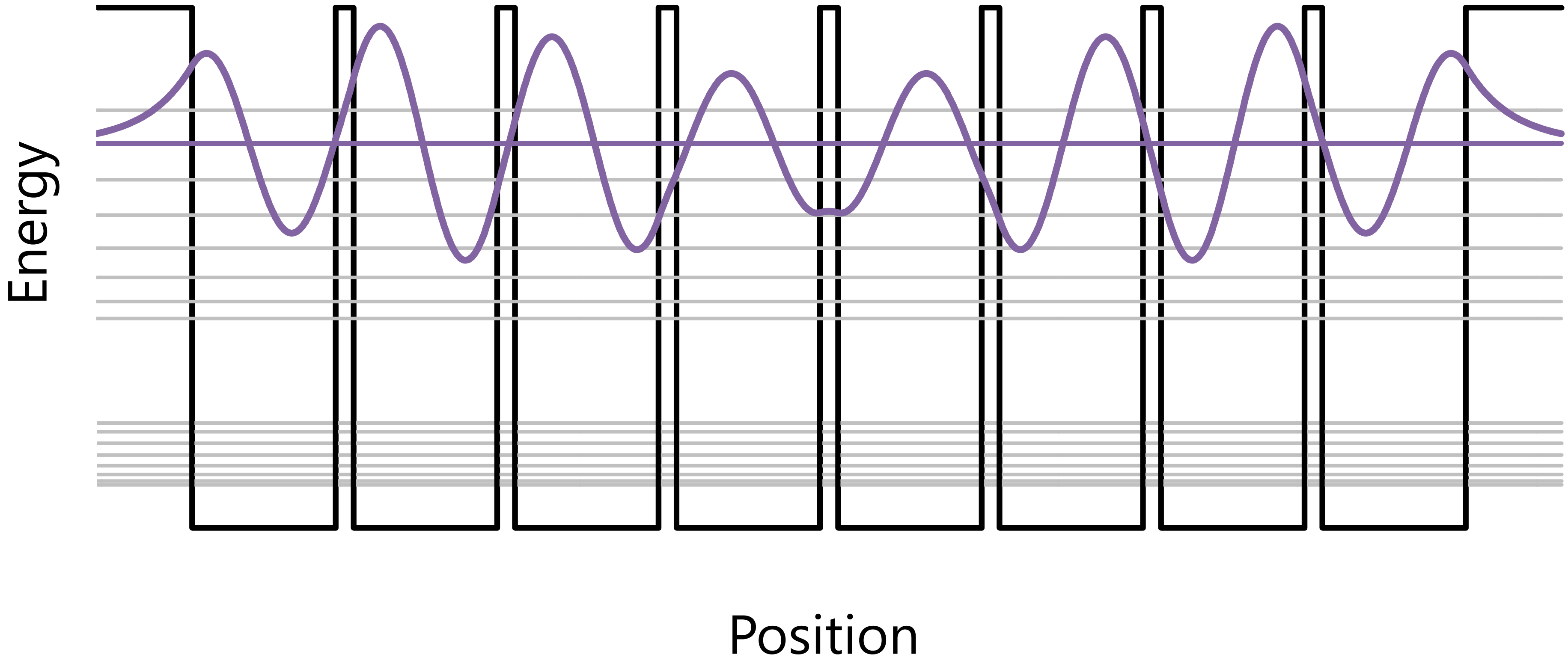

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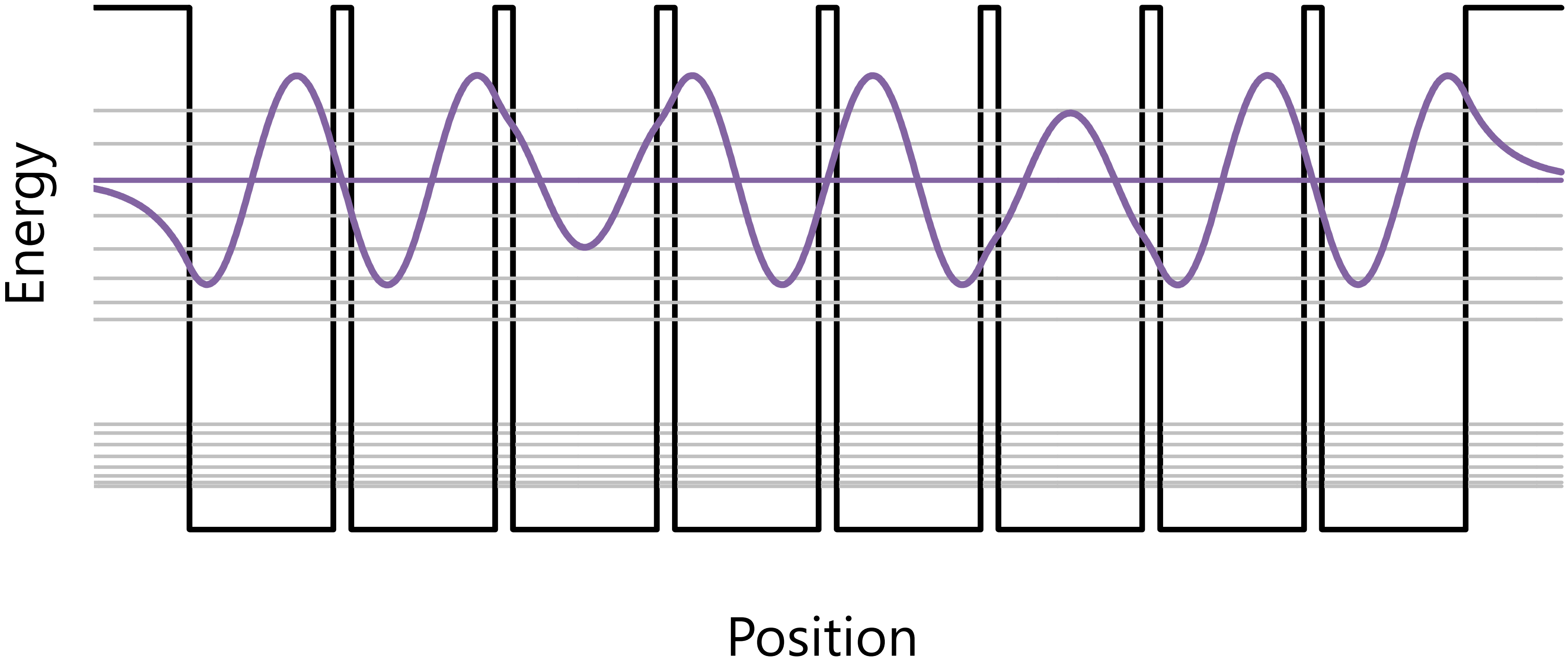

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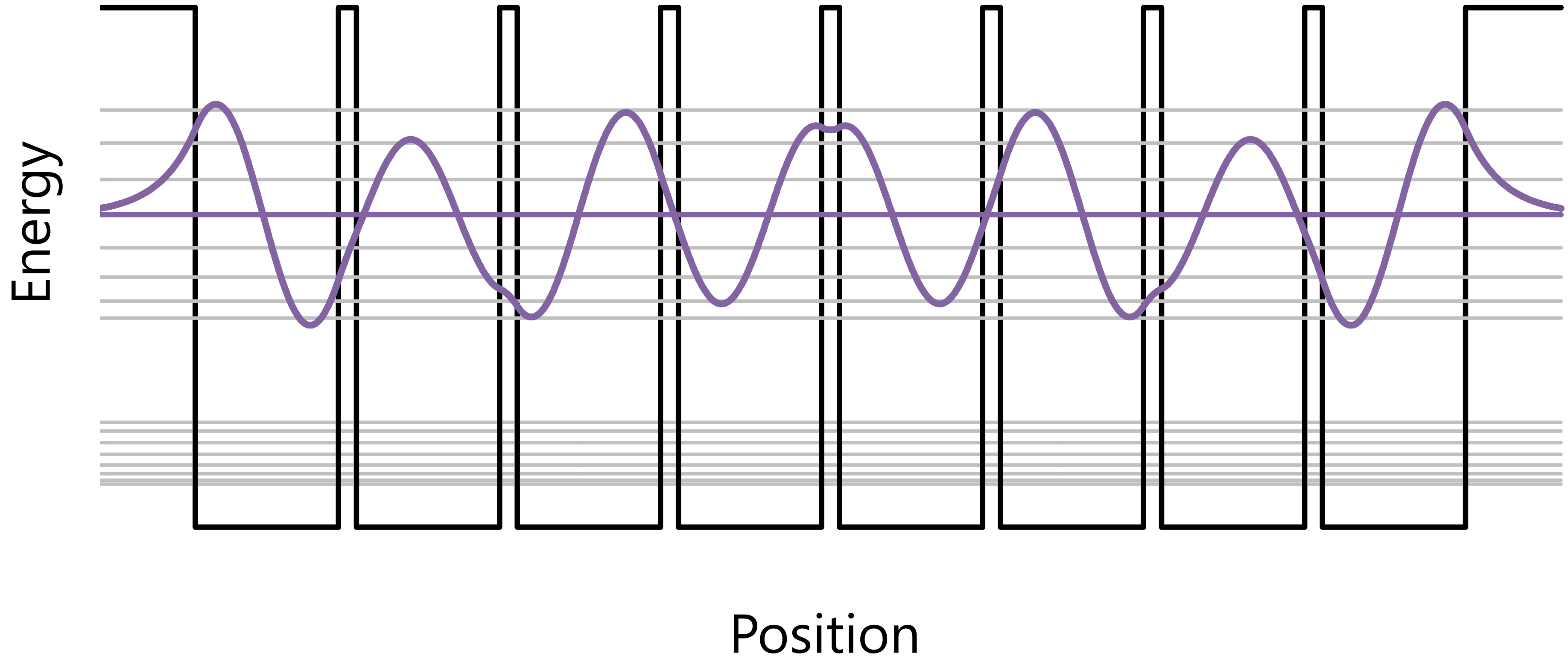

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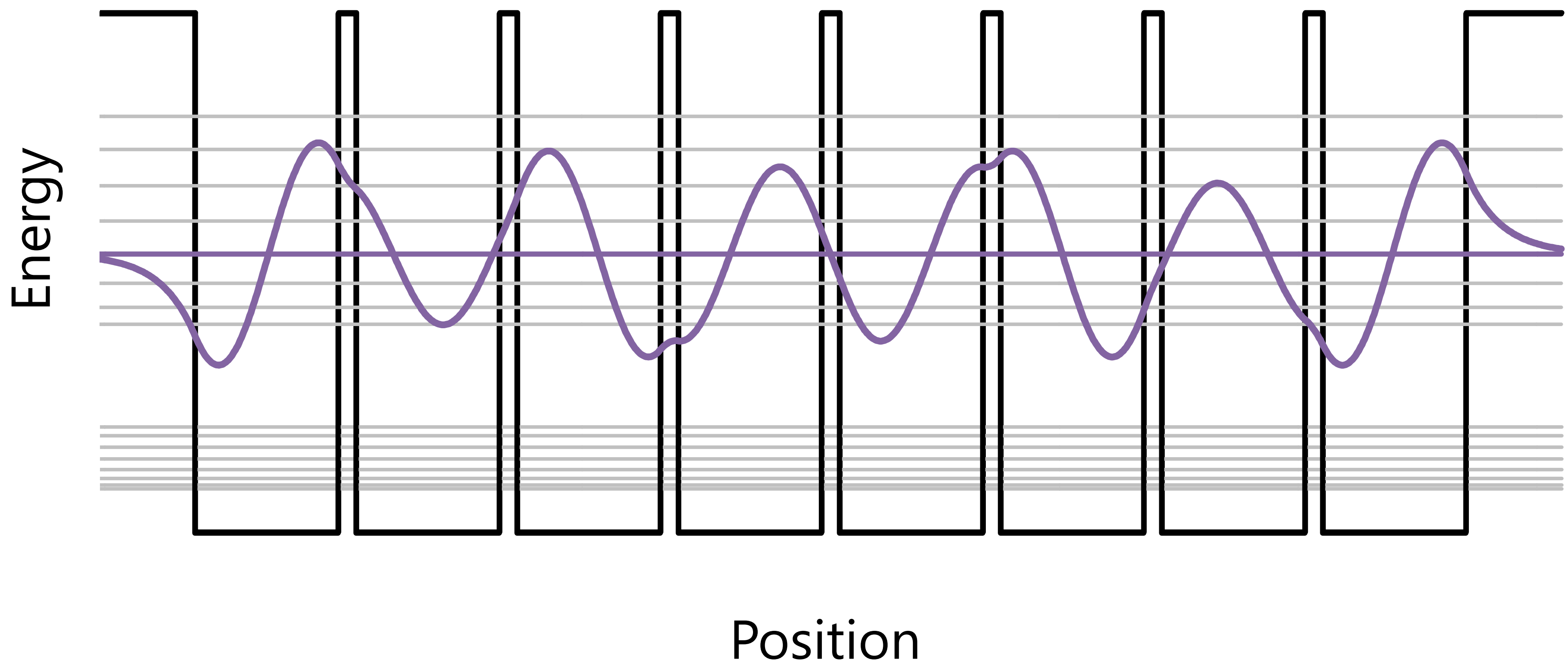

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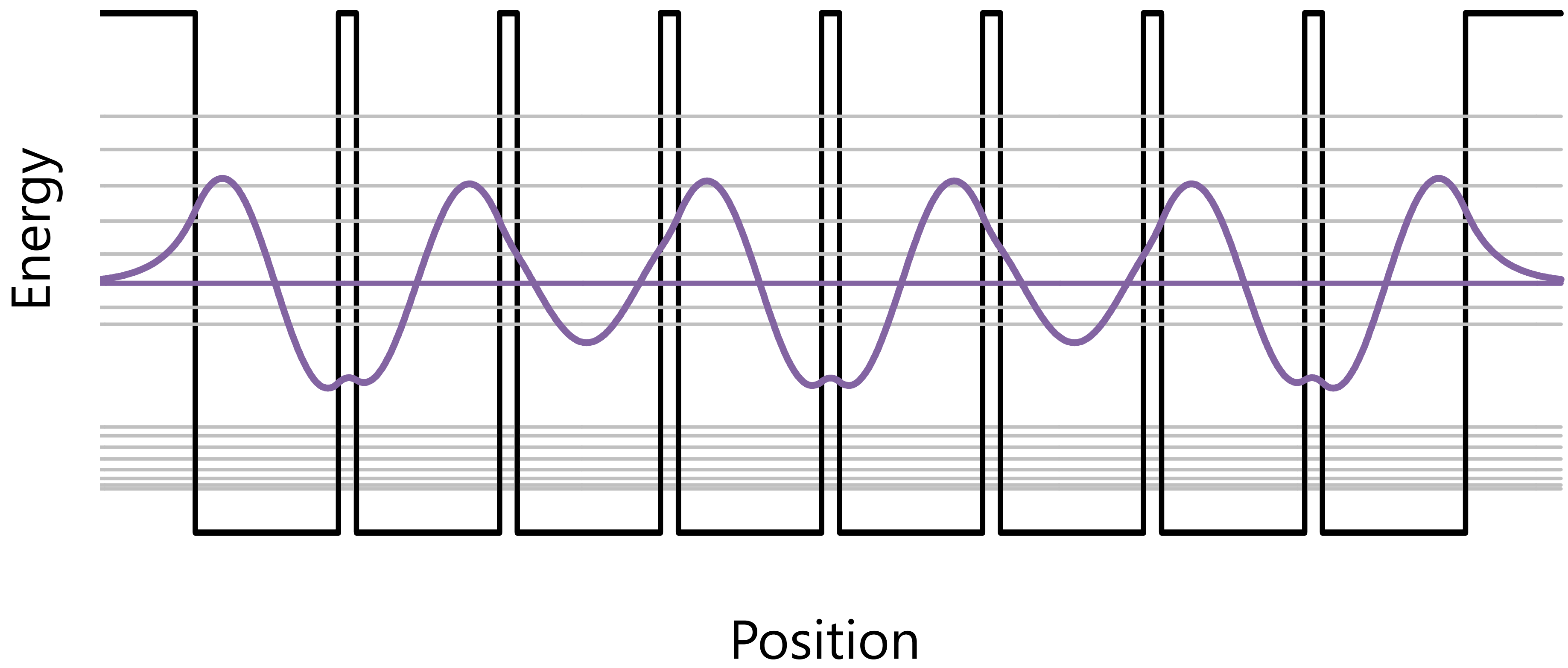
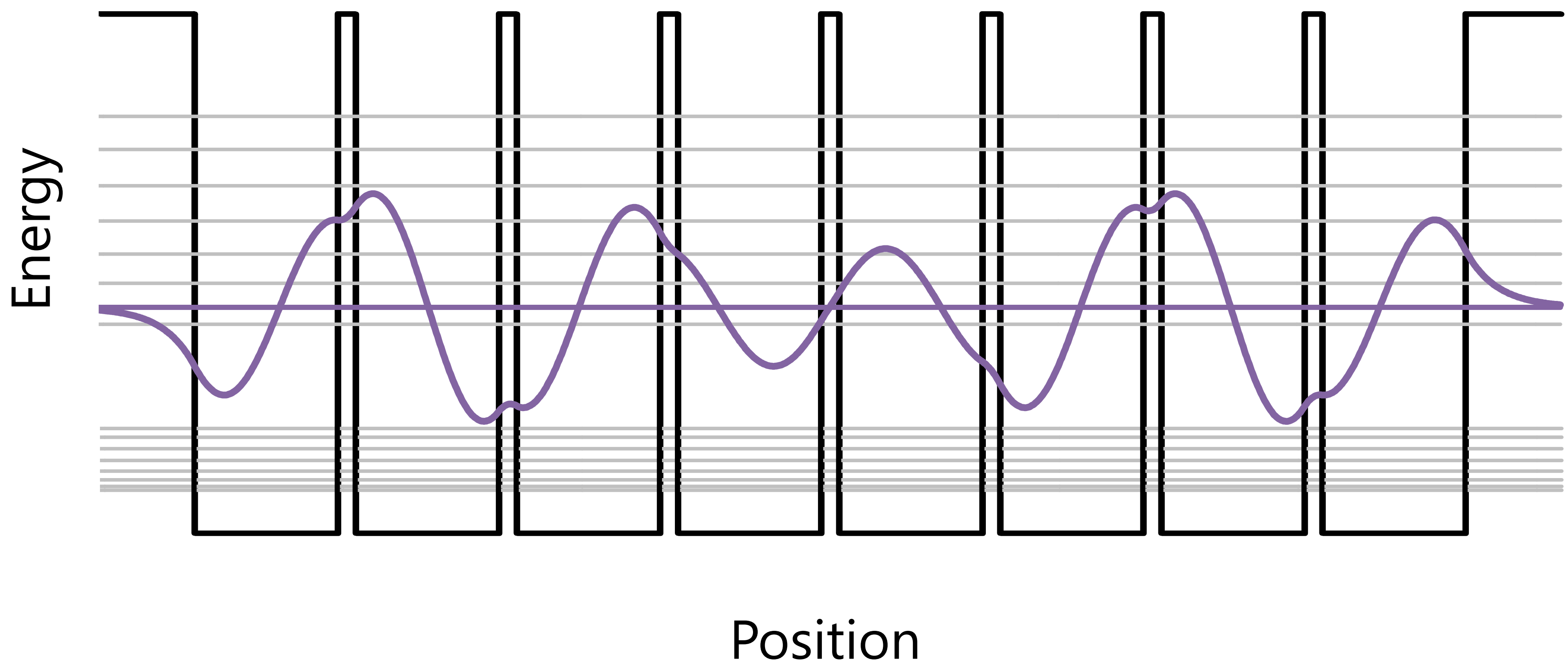
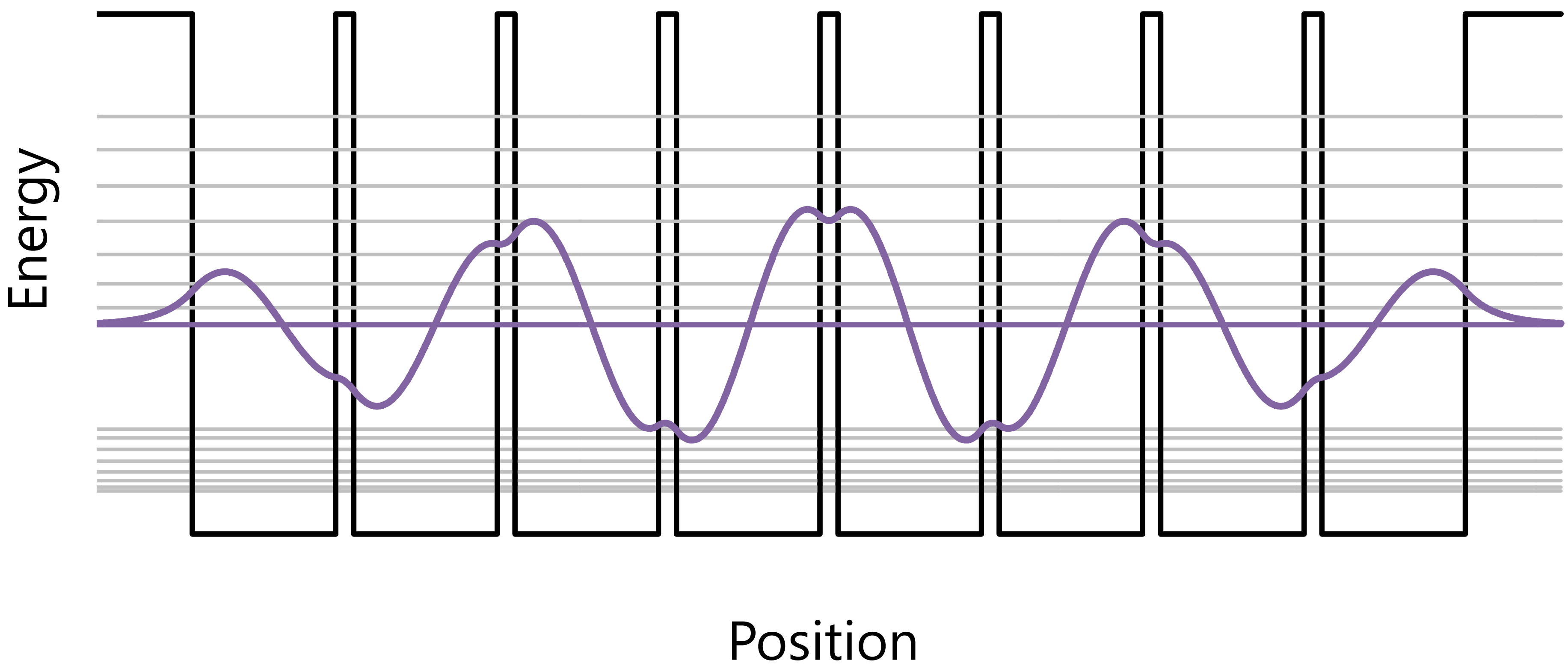


States for 8 coupled wells



States for 8 coupled wells



Multiple wells with multiple bands

If we increased the number of wells

- this same pattern of behavior would continue
  - just with correspondingly more levels
    - and more “half waves” in the envelope function
      - but still in the same “bands”
        - still with similar “unit cell” functions

Multiple wells with multiple bands

- The energy band "widths" would tend to saturate, with
  - a nearly flat "envelope" at one extreme of the band
  - a nearly "alternating" envelope at the other extreme