Physics 280 Quantum Mechanics Lecture II

Summer 2016

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Objectives

- Review of Schrödinger's Wave Equation

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- Tunneling

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- The Schrödinger Equation for two identical particles.

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- The Schrödinger Equation for two identical particles.
- Electron shells, why can't you have 100 electrons in the ground state?
- Quantum Mechanics explains why all metals aren't conductors.

Schrödinger's Wave Equation

- $$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + U\Psi(x,t) = i\hbar\frac{\partial\Psi(x,t)}{\partial t}$$

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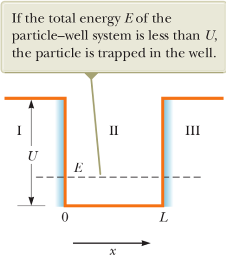
- And we can express it in three dimensions:
- $$-\frac{\hbar^2}{2m}\left(\frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2} + \frac{d^2\psi}{dz^2}\right) + U\psi = E\psi$$

Schrödinger's Wave Equation: Example



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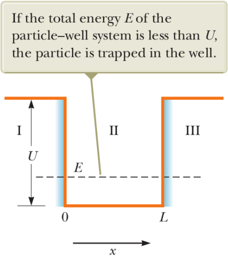

In regions I and III:

$$\frac{d^2\psi}{dx^2} = \frac{2m(U-E)}{\hbar^2}\psi \equiv C^2\psi$$

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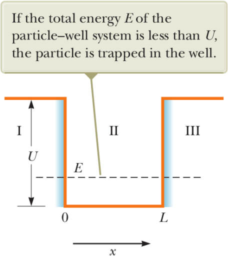


In regions I and III:

$$\frac{d^2\psi}{dx^2} = \frac{2m(U-E)}{\hbar^2}\psi \equiv C^2\psi$$

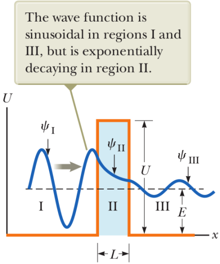
and in region II:

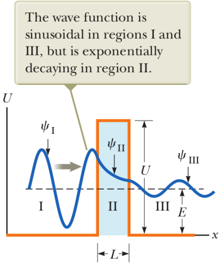
$$\frac{d^2\psi}{dx^2} = \frac{2mE}{\hbar^2}\psi$$

With solutions

$$\psi_I = Ae^{Cx},\ \psi_{II} = F\sin kx + G\cos kx,\ \psi_{III} = Be^{-Cx}$$

Tunneling


The wave function is sinusoidal in regions I and III, but is exponentially decaying in region II.
U
ψ I
ψ II
ψ III
U
E
I
II
III
x
L

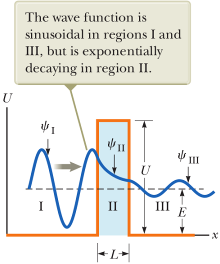


Recall that

$$C = \sqrt{\frac{2m(U - E)}{\hbar^2}}$$

It can be shown that the probability of an object tunneling through a barrier is:

Tunneling



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$$T \approx e^{-2CL}$$

Tunneling example

Q: A 30-eV electron is incident on a square barrier of height 40 eV and width 0.10 nm. You measure its location. You repeat this 10,000 times total. How many times to you expect that you'll find an electron on the other side of a barrier that classically it should be able to get beyond? $\hbar = 1.055 \times 10^{-34} Js$. 1eV $= 1.6 \times 10^{-19}$J. $m_e = 9.11 \times 10^{-31}$ kg .

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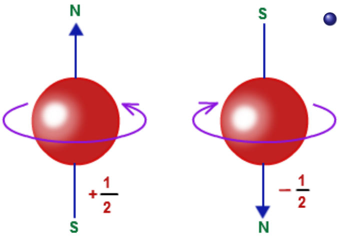
With 10,000 trials, you would expect to find about 390 incidents in which the electron tunneled through a barrier–which classical physics says is impossible.

Pauli Exclusion Principle



- An electron has intrinsic angular momentum, called **spin**. The image pictured at left is a classical model, **not** a quantum one. As far as we know, the electron is super super close to being a point particle.

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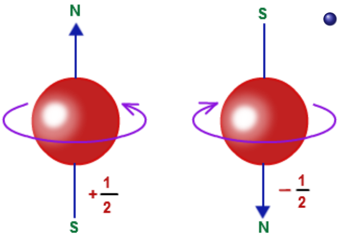

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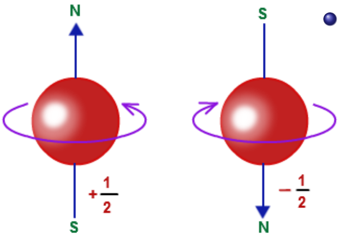

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- For an electron, the spin can be manifested as one of two types: spin up and spin down.
- The wave function for an electron needs to include its spin: $\psi(x) \rightarrow \psi(x) \uparrow or \psi(x) \downarrow$

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If there is a 30% chance of it raining tomorrow, and a 10% chance that your phone will fall tomorrow, what is the probability that it will both rain tomorrow and you will drop your phone?

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When a, b are independent.
So there is a 0.3(0.1) = 0.03 or 3
What does that *really* mean?

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It means that if there were 10,000 exact universes like ours with 10,000 yous, about 300 of yous would experience the heartbreak of a dropped phone while it is raining. Of course, it may be 288 or 380 or even 753 or 62, but the point is that the more duplicate universes you counted, the closer the number would get to 3%.

Pauli Exclusion Principle

Because the Schrödinger equation is a differential equation, solutions can be combined to yield equally valid solutions. Consider two particles, 1 and 2, which can exist in states a or b: $\psi_a(x_1)$, $\psi_b(x_2)$, $\psi_a(x_2)$, and $\psi_b(x_1)$. The functions we can form turn out to correspond to two distinct types of particles:

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$$\psi_{1,2}(x) = A\left(\psi_a(x_1)\psi_b(x_2) + \psi_b(x_1)\psi_a(x_2)\right) \quad \text{Bosons}$$

$$\psi_{1,2}(x) = B\left(\psi_a(x_1)\psi_b(x_2) - \psi_b(x_1)\psi_a(x_2)\right) \quad \text{Fermions}$$

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For Fermions, the wave function goes to zero if the particles are in the exact same states ($\psi_a = \psi_b$).

Two identical fermion particles can not inhabit the exact same quantum state.

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Electrons are fermions. Why can't we fit a hundred electrons into the ground state of a hydrogen atom? How many can we fit?

Because electrons have intrinsic spin, either spin up or spin down, an electron in the ground state of a particular hydrogen atom can be distinguished from another electron in the ground state of that same atom if and only if they have opposite spins. Thus each energy level can contain two electrons and only two electrons so long as they have opposite spin.

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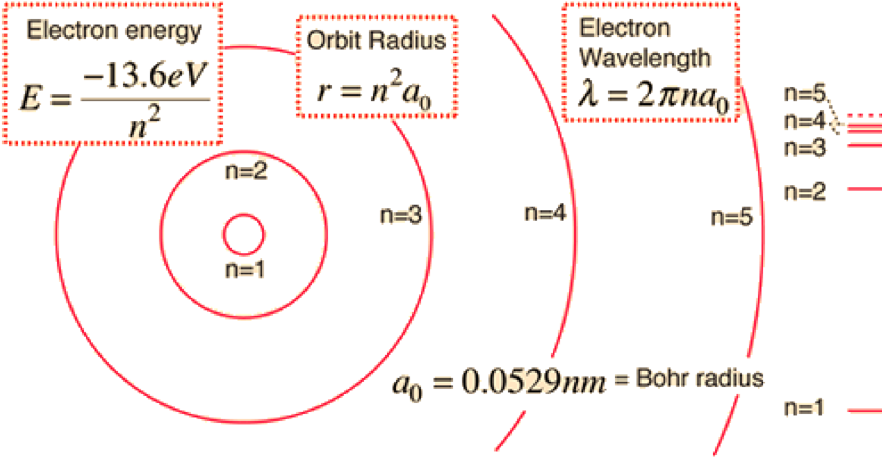
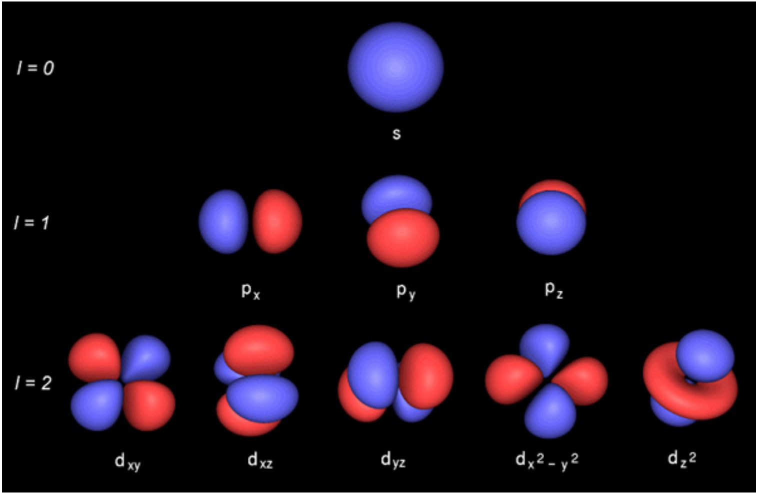
This **Pauli Exclusion Principle** is just one example of how *mathematics* is manifested in our *physical* universe. We will now look at another example of this manifestation.

Wrong:


Electron energy
$E = \frac{-13.6eV}{n^2}$
Orbit Radius
$r = n^2 a_0$
Electron
Wavelength
$\lambda = 2\pi n a_0$
n=1
n=2
n=3
n=4
n=5
n=5
n=4
n=3
n=2
n=1
$a_0 = 0.0529nm$ = Bohr radius

Right:



Periodic Table

Atom	1s	2s	2p			Electronic configuration
Li	↑↓	↑				$1s^2 2s^1$
Be	↑↓	↑↓				$1s^2 2s^2$
B	↑↓	↑↓	↑			$1s^2 2s^2 2p^1$
C	↑↓	↑↓	↑	↑		$1s^2 2s^2 2p^2$
N	↑↓	↑↓	↑	↑	↑	$1s^2 2s^2 2p^3$
O	↑↓	↑↓	↑↓	↑	↑	$1s^2 2s^2 2p^4$
F	↑↓	↑↓	↑↓	↑↓	↑	$1s^2 2s^2 2p^5$
Ne	↑↓	↑↓	↑↓	↑↓	↑↓	$1s^2 2s^2 2p^6$

Periodic Table

I	II											III	IV	V	VI	VII	0
H 1 $1s^1$																H 1 $1s^1$	He 2 $1s^2$
Li 3 $2s^1$	Be 4 $2s^2$											B 5 $2p^1$	C 6 $2p^2$	N 7 $2p^3$	O 8 $2p^4$	F 9 $2p^5$	Ne 10 $2p^6$
Na 11 $3s^1$	Mg 12 $3s^2$											Al 13 $3p^1$	Si 14 $3p^2$	P 15 $3p^3$	S 16 $3p^4$	Cl 17 $3p^5$	Ar 18 $3p^6$
K 19 $4s^1$	Ca 20 $4s^2$	Sc 21 $3d^1 4s^2$	Ti 22 $3d^2 4s^2$	V 23 $3d^3 4s^2$	Cr 24 $3d^5 4s^1$	Mn 25 $3d^5 4s^2$	Fe 26 $3d^6 4s^2$	Co 27 $3d^7 4s^2$	Ni 28 $3d^8 4s^2$	Cu 29 $3d^{10} 4s^1$	Zn 30 $3d^{10} 4s^2$	Ga 31 $4p^1$	Ge 32 $4p^2$	As 33 $4p^3$	Se 34 $4p^4$	Br 35 $4p^5$	Kr 36 $4p^6$
Rb 37 $5s^1$	Sr 38 $5s^2$	Y 39 $4d^1 5s^2$	Zr 40 $4d^2 5s^2$	Nb 41 $4d^4 5s^1$	Mo 42 $4d^5 5s^1$	Tc 43 $4d^5 5s^2$	Ru 44 $4d^7 5s^1$	Rh 45 $4d^8 5s^1$	Pd 46 $4d^{10}$	Ag 47 $4d^{10} 5s^1$	Cd 48 $4d^{10} 5s^2$	In 49 $5p^1$	Sn 50 $5p^2$	Sb 51 $5p^3$	Te 52 $5p^4$	I 53 $5p^5$	Xe 54 $5p^6$
Cs 55 $6s^1$	Ba 56 $6s^2$	57-71*	Hf 72 $5d^2 6s^2$	Ta 73 $5d^3 6s^2$	W 74 $5d^4 6s^2$	Re 75 $5d^5 6s^2$	Os 76 $5d^6 6s^2$	Ir 77 $5d^7 6s^2$	Pt 78 $5d^9 6s^1$	Au 79 $5d^{10} 6s^1$	Hg 80 $5d^{10} 6s^2$	Tl 81 $6p^1$	Pb 82 $6p^2$	Bi 83 $6p^3$	Po 84 $6p^4$	At 85 $6p^5$	Rn 86 $6p^6$
Fr 87 $7s^1$	Ra 88 $7s^2$	89-103**	Rf 104 $6d^2 7s^2$	Db 105 $6d^3 7s^2$	Sg 106 $6d^4 7s^2$	Bh 107 $6d^5 7s^2$	Hs 108 $6d^6 7s^2$	Mt 109 $6d^7 7s^2$	Ds 110 $6d^9 7s^1$	Rg 111	112		114		116		

*Lanthanide series	La 57 $5d^1 6s^2$	Ce 58 $5d^1 4f^1 6s^2$	Pr 59 $4f^3 6s^2$	Nd 60 $4f^4 6s^2$	Pm 61 $4f^5 6s^2$	Sm 62 $4f^6 6s^2$	Eu 63 $4f^7 6s^2$	Gd 64 $5d^1 4f^7 6s^2$	Tb 65 $5d^1 4f^8 6s^2$	Dy 66 $4f^{10} 6s^2$	Ho 67 $4f^{11} 6s^2$	Er 68 $4f^{12} 6s^2$	Tm 69 $4f^{13} 6s^2$	Yb 70 $4f^{14} 6s^2$	Lu 71 $5d^1 4f^{14} 6s^2$
**Actinide series	Ac 89 $6d^1 7s^2$	Th 90 $6d^2 7s^2$	Pa 91 $5f^2 6d^1 7s^2$	U 92 $5f^3 6d^1 7s^2$	Np 93 $5f^4 6d^1 7s^2$	Pu 94 $5f^6 7s^2$	Am 95 $5f^7 7s^2$	Cm 96 $5f^7 6d^1 7s^2$	Bk 97 $5f^8 6d^1 7s^2$	Cf 98 $5f^{10} 7s^2$	Es 99 $5f^{11} 7s^2$	Fm 100 $5f^{12} 7s^2$	Md 101 $5f^{13} 7s^2$	No 102 $5f^{14} 7s^2$	Lr 103 $5f^{14} 6d^1 7s^2$

Band Structure

Mystery:
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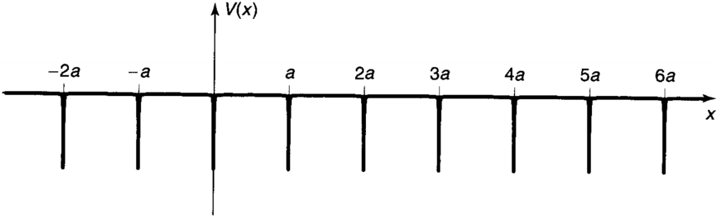
Why are some materials insulators and other materials conductors?

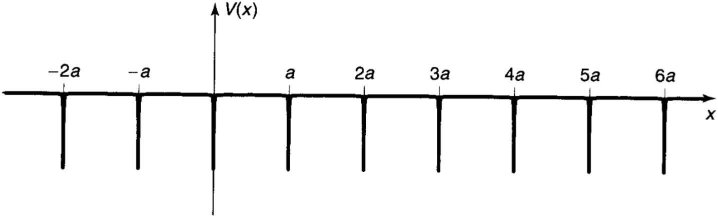
Band Structure

Dirac Comb:



Models materials as a ”comb” of infinite potentials (the nucleus).

Band Structure



- The potential is periodic $V(x+a) = V(x)$.

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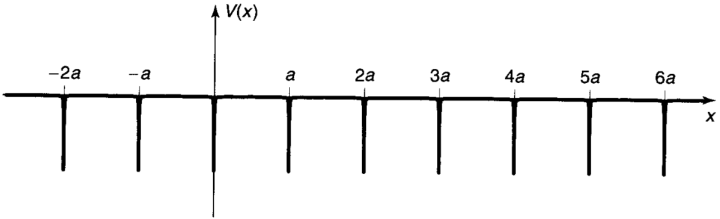

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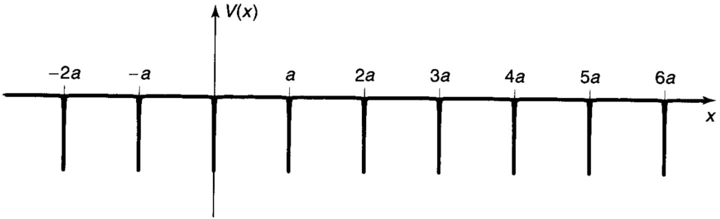

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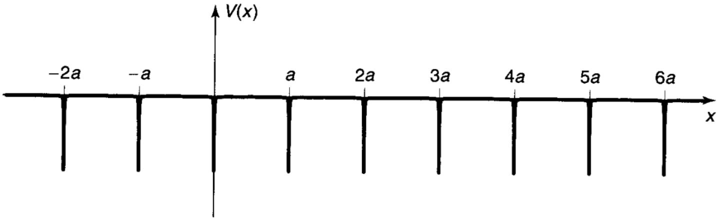

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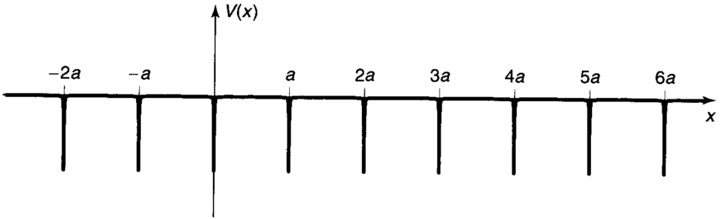
- Cell to right of origin:
  $\psi(x) = A\sin(kx) + B\cos(kx),\ 0 < x < a,\ k = \frac{\sqrt{2mE}}{\hbar}$

Band Structure



- The potential is periodic $V(x+a) = V(x)$.
- Bloch's theorem gives $\psi(x+a) = e^{iKa}\psi(x)$ where K is a constant and i represents $\sqrt{-1}$
- Let's focus on the solution for the block just to the left and right of the origin.
- Cell to right of origin:
  $\psi(x) = A\sin(kx) + B\cos(kx),\ 0 < x < a,\ k = \frac{\sqrt{2mE}}{\hbar}$
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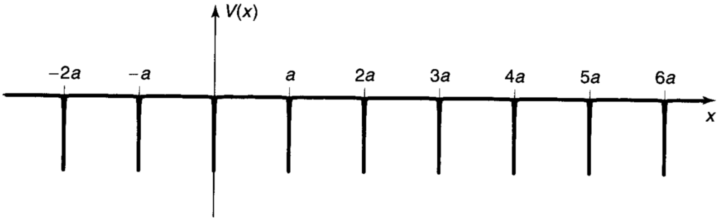
Band Structure



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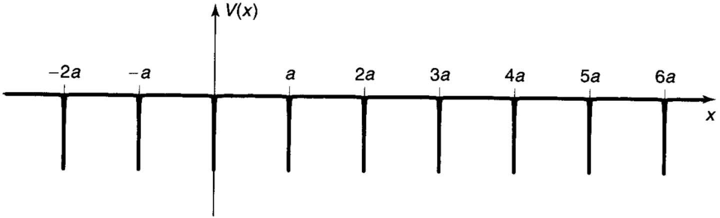

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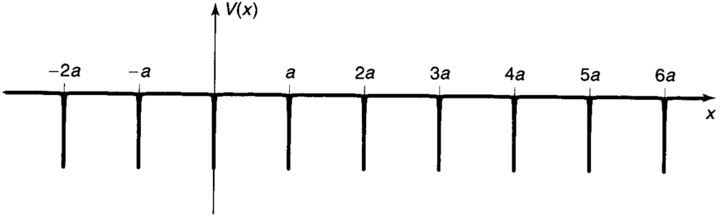
These equations must be continuous at their intersection $x = 0$. This yields the conditions:

$$B = e^{iKa}\left[A\sin(ka) + B\cos(ka)\right]$$

Band Structure

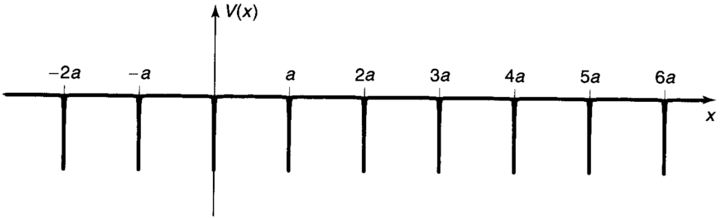


The derivatives must also be continues which yields:

$$kA - e^{-iKa}k\left[A\cos(ka) - B\sin(ka)\right] = -\frac{2m\alpha}{\hbar^2}B$$

where α is a constant depending on the material.

Band Structure



These two continuity conditions can be merged to yield:

$$\cos(Ka) = \cos(ka) - \frac{m\alpha}{\hbar^2 k}\sin(ka)$$

Note that thus far this is just a mathematical result, but it has interesting implications.

Band Structure

Let $z = ka$ and $\beta = \frac{m\alpha a}{\hbar^2}$ so that the continuity condition can be written:

$$f(z) = \cos(z) - \beta\frac{\sin(z)}{z}$$

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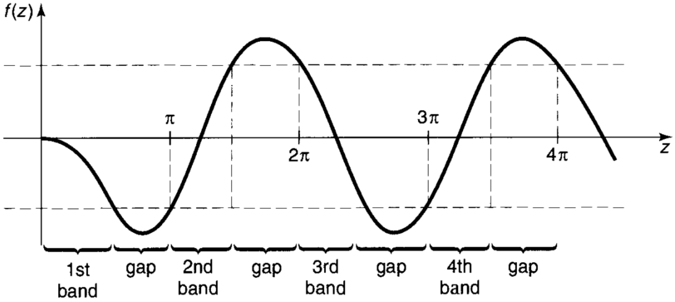

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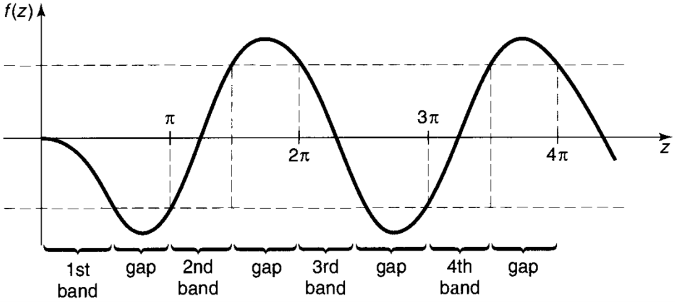
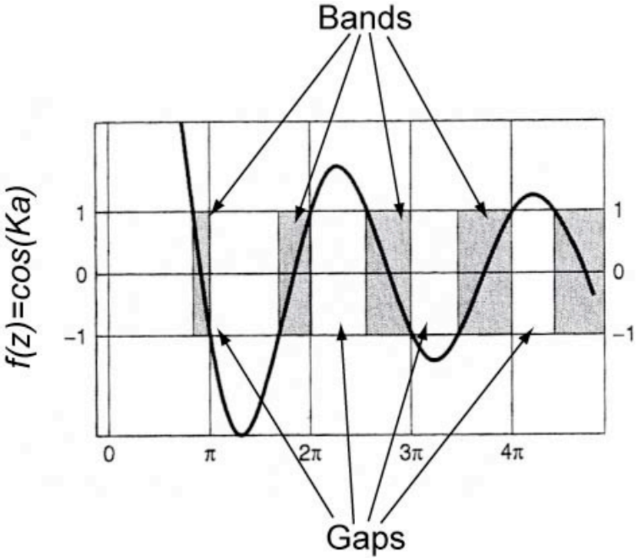


Can you spot the problem?

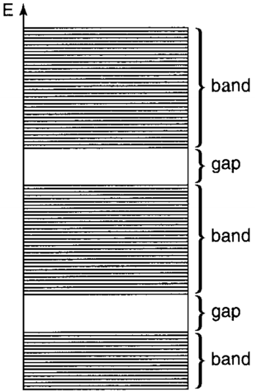
Band Structure

Since $|\cos(Ka)| \leq 1$, the equation only "works" in certain "bands":



Band Structure

This corresponds to areas in the Energy "spectrum" which can never be occupied:



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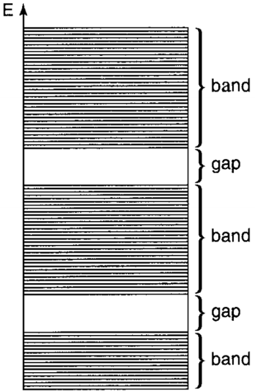

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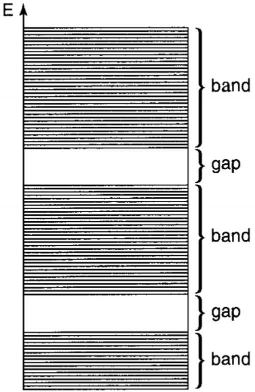

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- Electrons in these bands must make a quantum leap to higher energy bands but can never have energy equal to anywhere in the gap.
- If a gap is completely filled, takes a lot more energy to excite an electron to the next higher energy state since it has to "jump" across gap.

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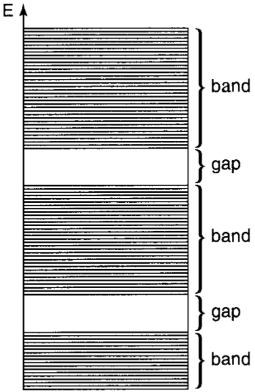

- In some materials, the lowest bands completely occupied with the material’s electrons already and it takes a lot of energy to jump the gap. These metals are insulators.

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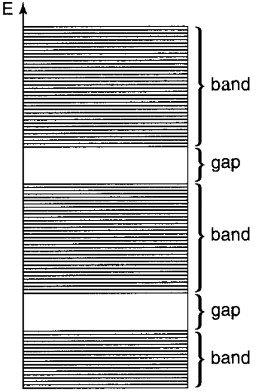

- In some materials, the lowest bands completely occupied with the material's electrons already and it takes a lot of energy to jump the gap. These metals are insulators.
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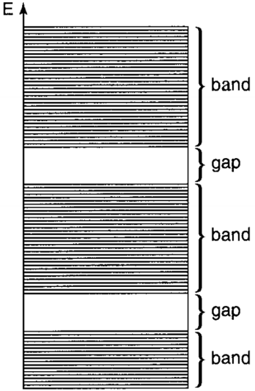

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- In other materials, the highest occupied band has room for more electrons and so it is easy to excite those electrons to higher energy states. These are conductors.
- ”Doping” of insulators can lead to semiconductors where either electrons are now in the next higher band or holes are in the previously filled one, and so weak currents can flow.

Mystery:
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Quantum Mechanics solves this mystery precisely! The solution shows us how deeply mathematics dictates the physical manifestation of the universe.