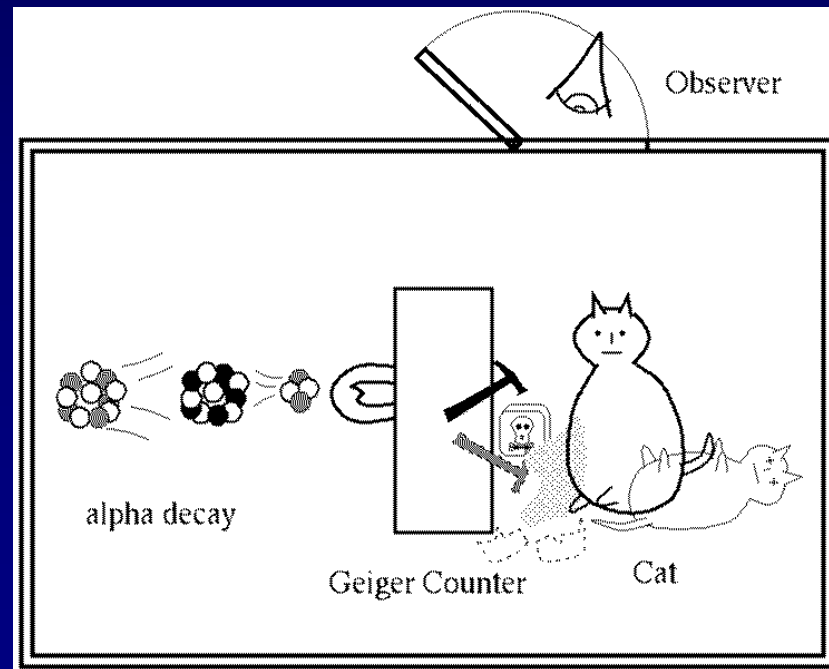
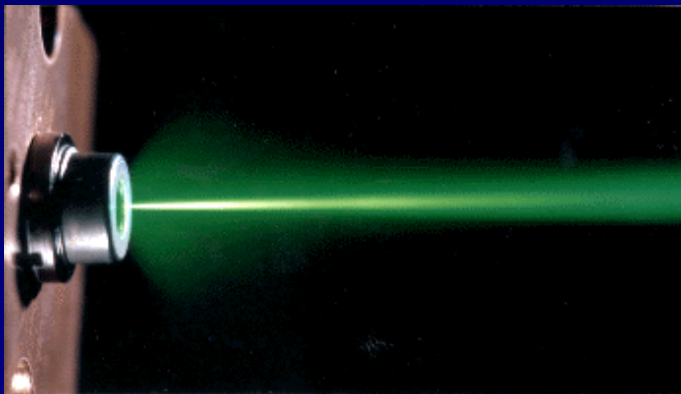


"When I hear of  
Schrödinger's cat, I  
reach for my gun."

--Stephen W.  
Hawking



# Lecture 21: Lasers, Schrödinger's Cat, Atoms, Molecules, Solids, etc. Review and Examples



# Act 1

The Pauli exclusion principle applies to all fermions in all situations (not just to electrons in atoms). Consider electrons in a 2-dimensional infinite square well potential.

1. How many electrons can be in the first excited energy level?  
a. 1    b. 2    c. 3    d. 4    e. 5

Hint: Remember the  $(n_x, n_y)$  quantum numbers.

2. If there are 4 electrons in the well, what is the energy of the most energetic one (ignoring e-e interactions, and assuming the total energy is as low as possible)?
- a.  $(h^2/8mL^2) \times 2$   
b.  $(h^2/8mL^2) \times 5$   
c.  $(h^2/8mL^2) \times 10$

# Solution

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1. How many electrons can be in the first excited energy level?  
a. 1    b. 2    c. 3    **d. 4**    e. 5

The first excited energy level has  $(n_x, n_y) = (1, 2)$  or  $(2, 1)$ .

That is, it is degenerate.

Each of these can hold two electrons (spin up and down).

(Note: On an exam, I'd word this question a bit more carefully.)

2. If there are 4 electrons in the well, what is the energy of the most energetic one (ignoring e-e interactions, and assuming the total energy is as low as possible)?

- a.  $(h^2/8mL^2) \times 2$   
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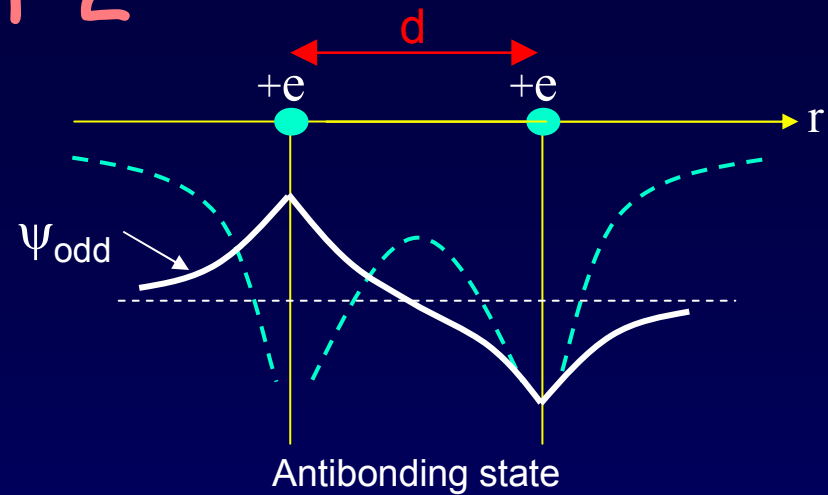
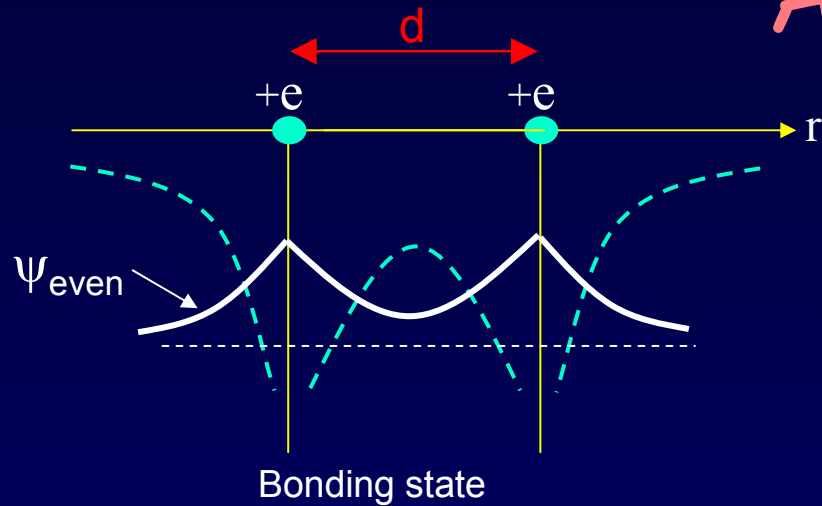
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**b.  $(h^2/8mL^2) \times 5$**   
c.  $(h^2/8mL^2) \times 10$

Two electrons are in the  $(1, 1)$  state, and two are in the  $(2, 1)$  or  $(1, 2)$  state. So,  $E_{\max} = (1^2 + 2^2) \times (h^2/8mL^2)$ .

# Act 2

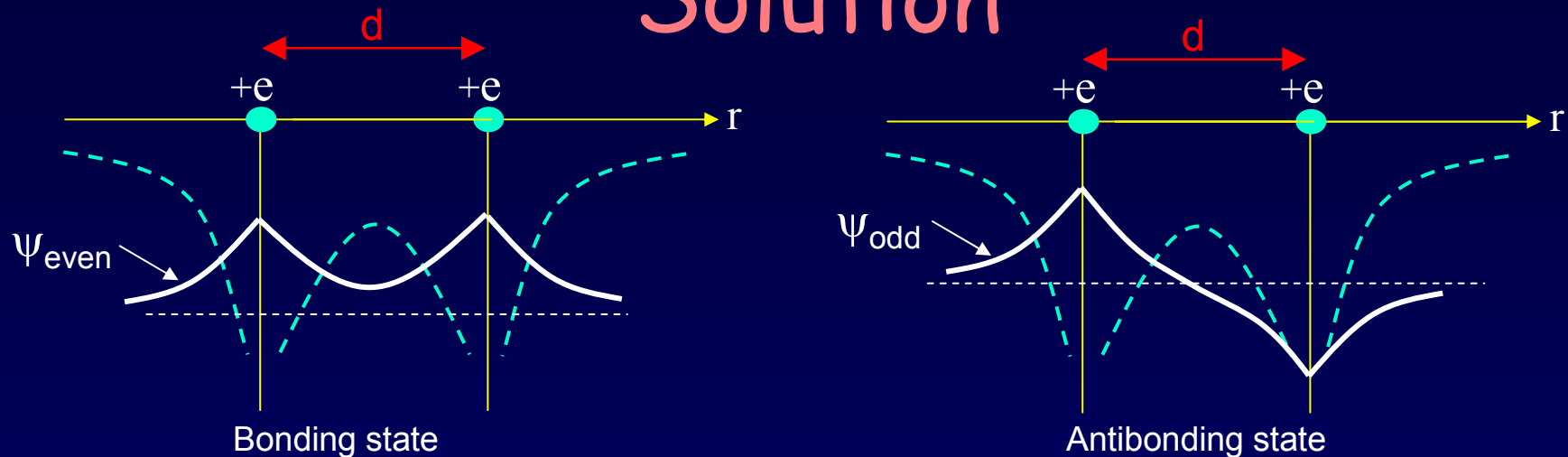


As  $d$  decreases, the energy of the bonding state decreases (until a minimum energy is reached), while that of the antibonding state does not.

The reason is:

- The nuclei have a stronger interaction in the bonding state.
- The bonding state spreads out more, i.e., has less curvature.
- The electron is a fermion, and prefers the symmetric  $\psi$ .

# Solution



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- The electron is a fermion, and prefers the symmetric  $\psi$ .

- False. First, the interaction between the nuclei is *repulsive*. And in fact, this is somewhat shielded by the electron sitting in between, which actually reduces the repulsion (and lowers the energy).
- is right. The node in the antisymmetric state prevents the wavelength from increasing much. Also, in the bonding state the electron probability between the nuclei increases, “pulling” the nuclei toward it.
- The fact that the electron is a fermion is irrelevant. That only affects multi-electron states.

# Insulators, Semiconductors and Metals

Energy bands and the gaps between them determine the conductivity and other properties of solids.

## Insulators

Have a full valence band and a large energy gap (a few eV). Higher energy states are not available.

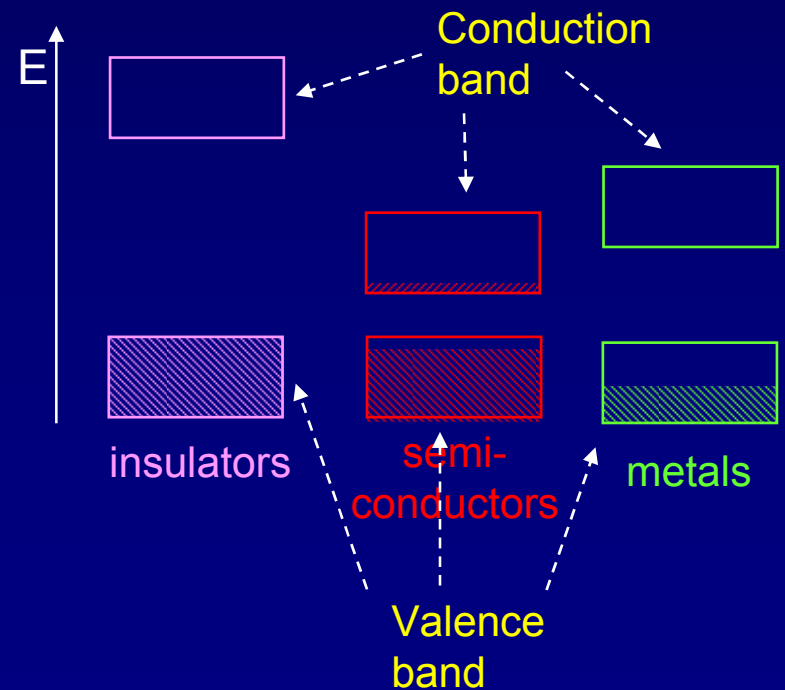
In order to conduct, an electron must have an available state at higher energy.

## Semiconductors

Are insulators at  $T = 0$ .  
Have a small energy gap ( $\sim 1$  eV) between valence and conduction bands. Higher energy states become available (due to  $kT$ ) as  $T$  increases.

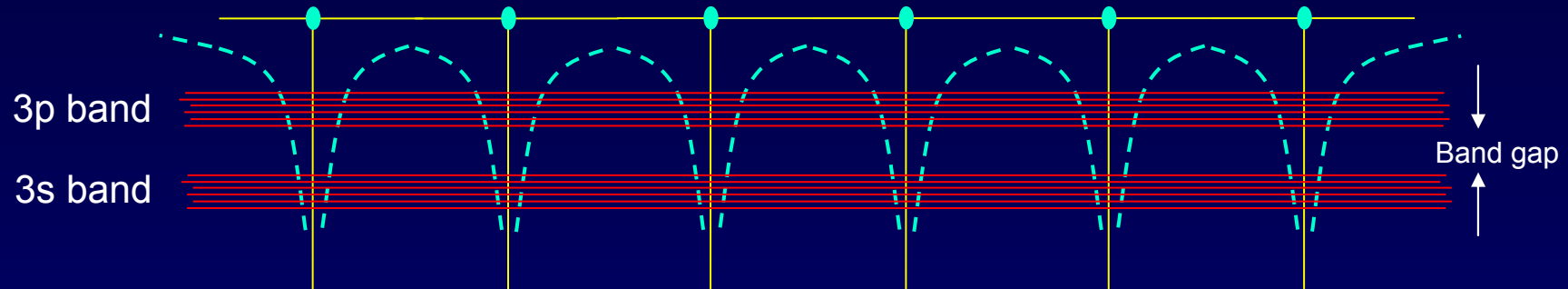
## Metals

Have a partly filled band. Higher energy states are available, even at  $T = 0$ .





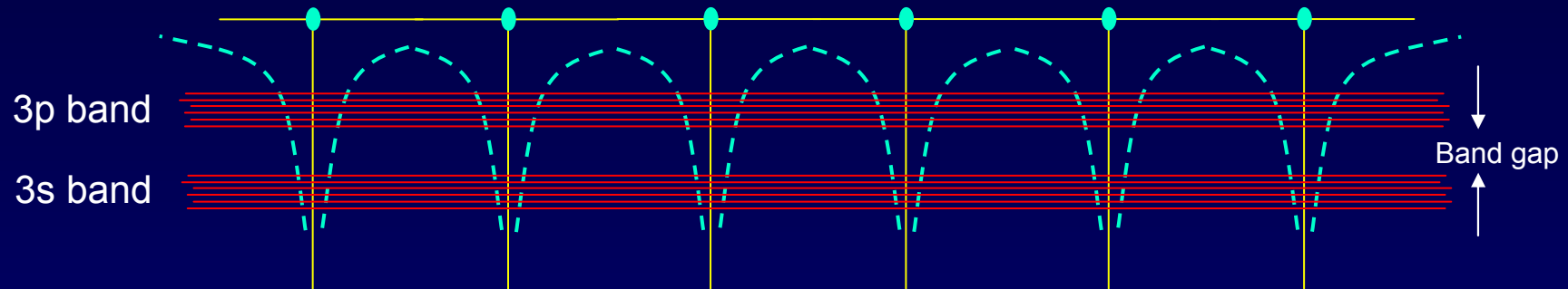
# Act 3



Consider a crystalline solid in which each atom contributes some electrons to the 3s band. Which situation can produce a conductor.

- Each atom contributes one 3s electron.
- Each atom contributes two 3s electrons.
- Each atom contributes three 3s electrons.

# Solution



Consider a crystalline solid in which each atom contributes some electrons to the 3s band. Which situation can produce a conductor.

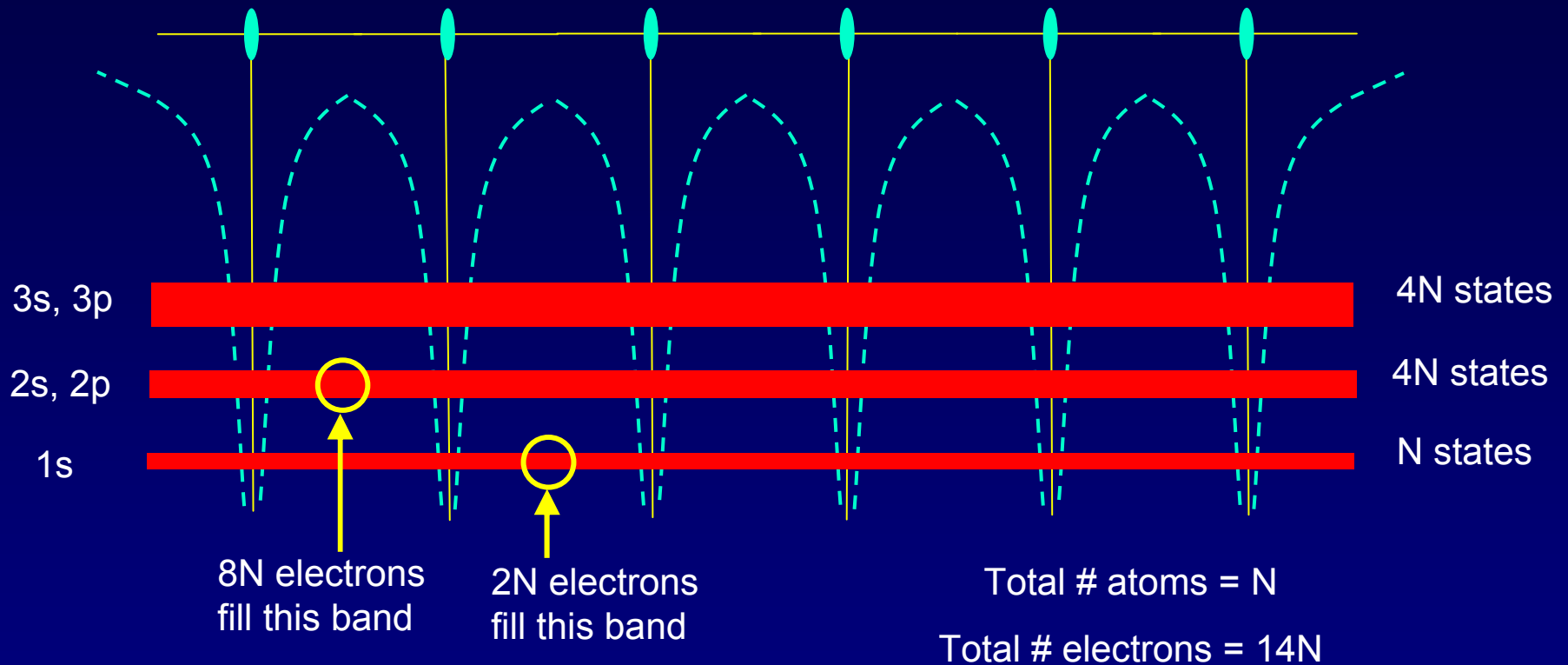
- a. Each atom contributes one 3s electron.
- b. Each atom contributes two 3s electrons.
- c. Each atom contributes three 3s electrons.

For  $N$  atoms, the band can hold  $2N$  electrons (spin up and spin down). So:

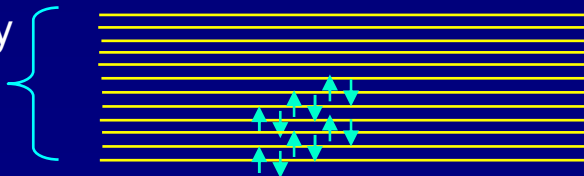
- a) gives us a half-filled band (conductor).
- b) gives a full band (insulator).
- c) is not possible. An atom can only have two 3s electrons.

# Semiconductors

Silicon:  $Z = 14$  ( $1s^2 2s^2 2p^6 3s^2 3p^2$ )



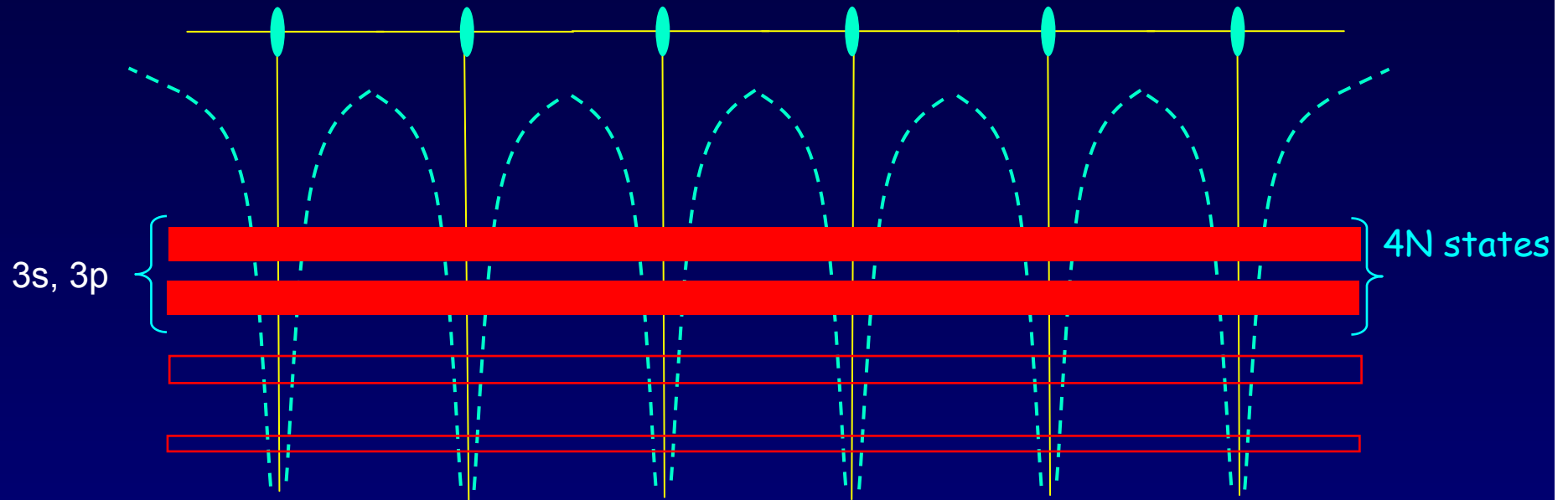
The 3s/3p band is only half filled (4N states and 4N electrons)



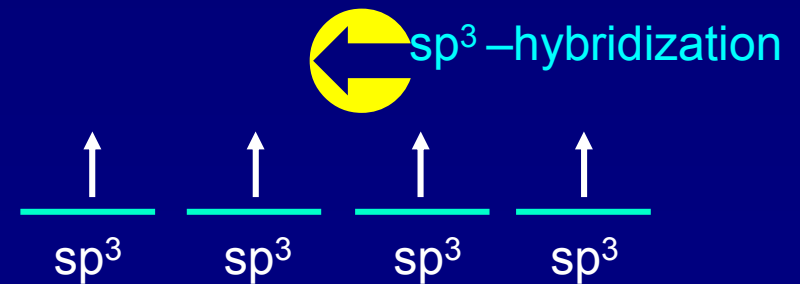
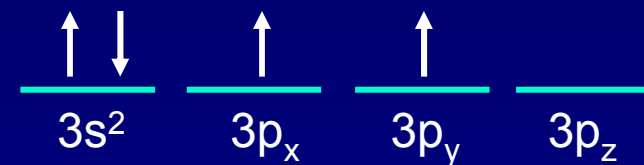
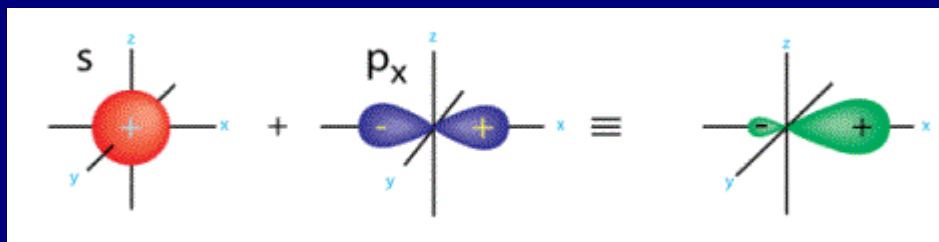
Why isn't Silicon a metallic conductor, like sodium?

# Energy Bands in Si

$$Z = 14: 1s^2 2s^2 2p^6 3s^2 3p^2$$

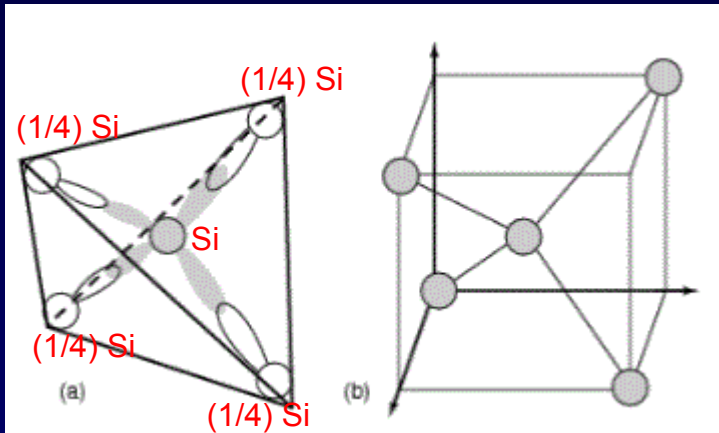


In Si, the  $3s^2$  and  $3p^2$  hybridize to form four equivalent  $sp^3$ -hybrid states. These eigenstates are linear combinations of s and p states:



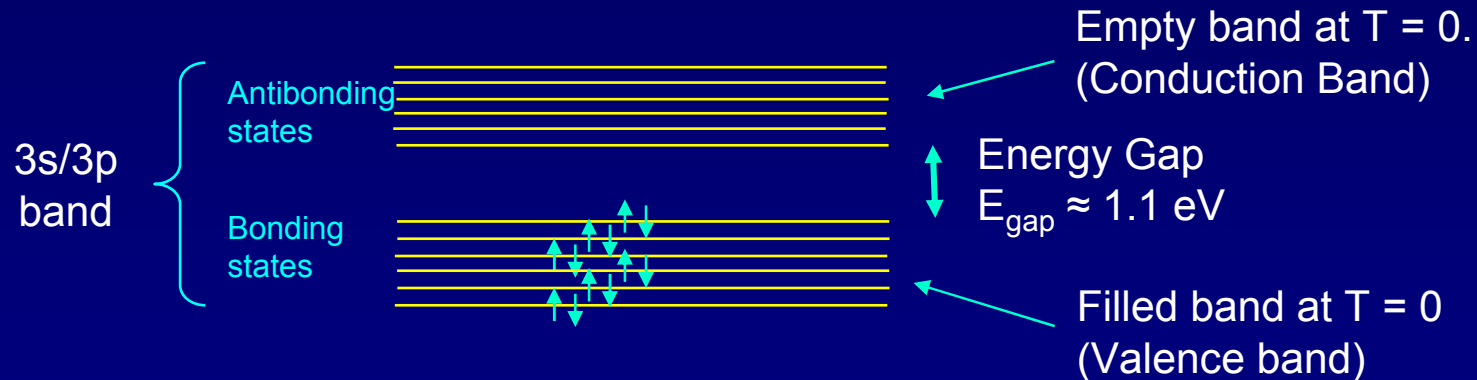
# Silicon (2)

## Silicon Unit Cell



2 - Si atoms/unit cell

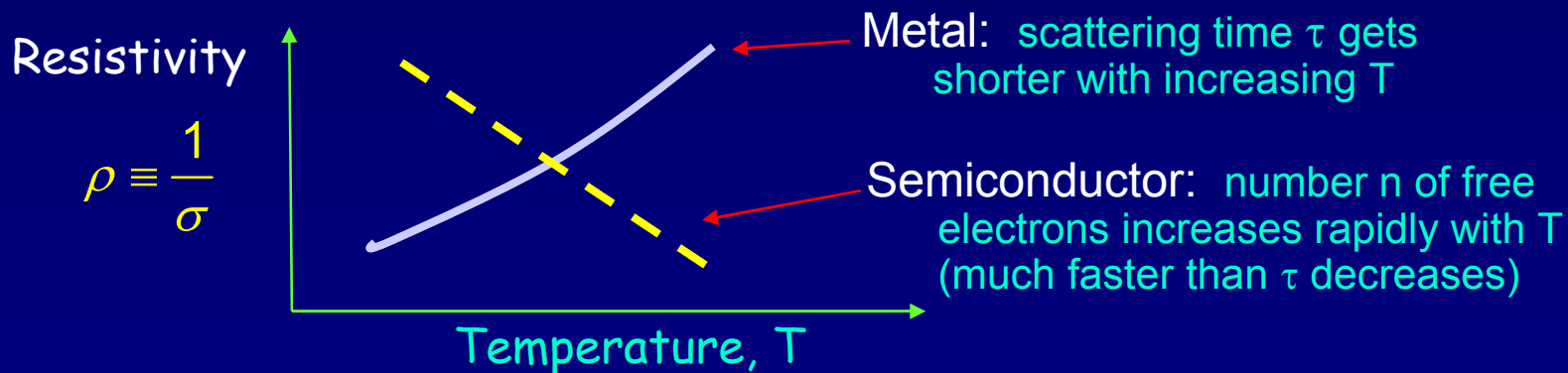
There are 2 types of superpositions between neighbors:



- ❑ 8  $sp^3$ -orbitals in one unit cell
- ❑ 8 orbitals form superpositions (4 bonding and 4 anti-bonding combinations)
- ❑ 8 orbitals  $\times$  2 spin = 16 states
- ❑ 8 electrons fill the 4 lower energy (bonding) states

# Silicon (3)

- At  $T = 0$ , the bonding states in Si are completely filled, and the anti-bonding states are completely empty. A small (1.1 eV) energy gap separates the bonding and anti-bonding states: Si is a semiconductor.
- The electrons in a filled band cannot contribute to conduction, because with reasonable E fields they cannot be promoted to a higher kinetic energy. Therefore, at  $T = 0$ , Si is an insulator. At higher temperatures, however, electrons are thermally promoted into the conduction band:



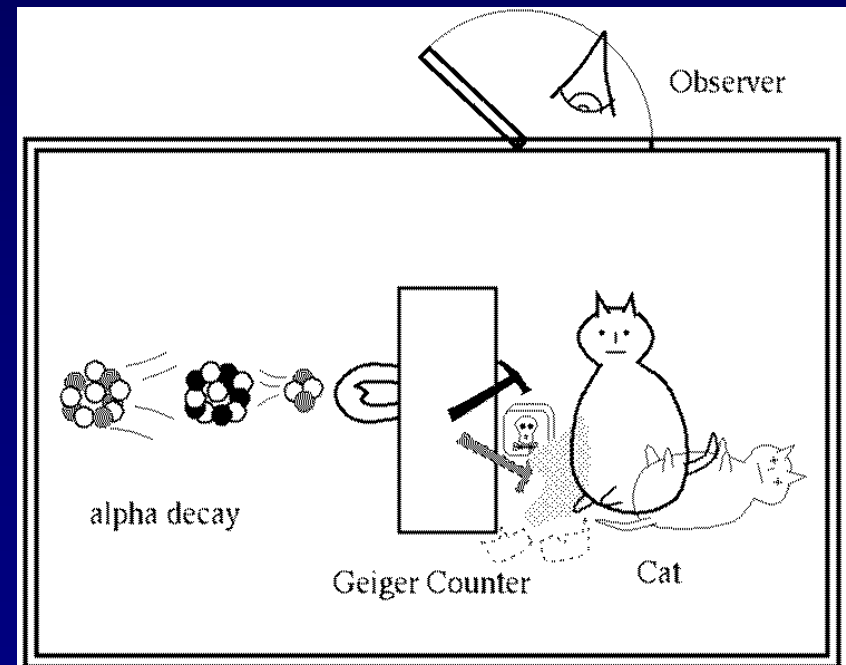
This graph only shows trends. A semiconductor has much higher resistance than a metal.

# Schrödinger's Cat:

## How seriously do we take superpositions?

- We now know that we can put a quantum object into a superposition of states.
- But if quantum mechanics is completely correct, shouldn't macroscopic objects end up in a superposition state too?
- This puzzle is best exemplified by the famous "Schrödinger's cat" paradox:
  - A radioactive nucleus can decay, emitting an alpha particle. This is a quantum mechanical process.
  - The alpha particle is detected with a Geiger counter, which releases a hammer, which breaks a bottle, which releases cyanide, which kills a cat.
  - Suppose we wait until there is a 50:50 chance that the nucleus has decayed.

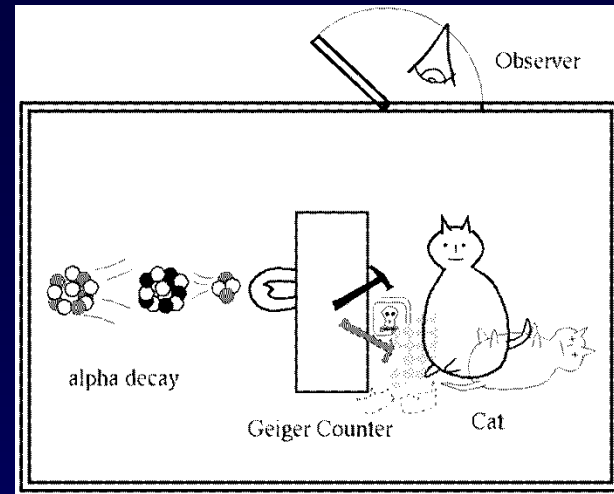
Is the cat alive or dead?



# Schrödinger's Cat

According to QM, because we can't know (*i.e.*, predict), until we look inside the box, the cat is in a superposition\* of being both alive and dead!

$$\Psi_{\text{cat}} = \frac{1}{\sqrt{2}} \{ \psi(\text{alive}) + \psi(\text{dead}) \}$$



And in fact, according to QM, when we look, we are put into a quantum superposition\* of having seen a live and a dead cat!!

Did you ever perceive yourself as being in a superposition? (probably not ...)

This paradox leads to some dispute over the applicability of QM to large objects. The experiments are difficult, but so far there is no evidence of a “size limit”.

Where does it end?!?

- it doesn't end (“wavefunction of the universe”)
- there is some change in physics (quantum → classical)
- “many-worlds” interpretation...

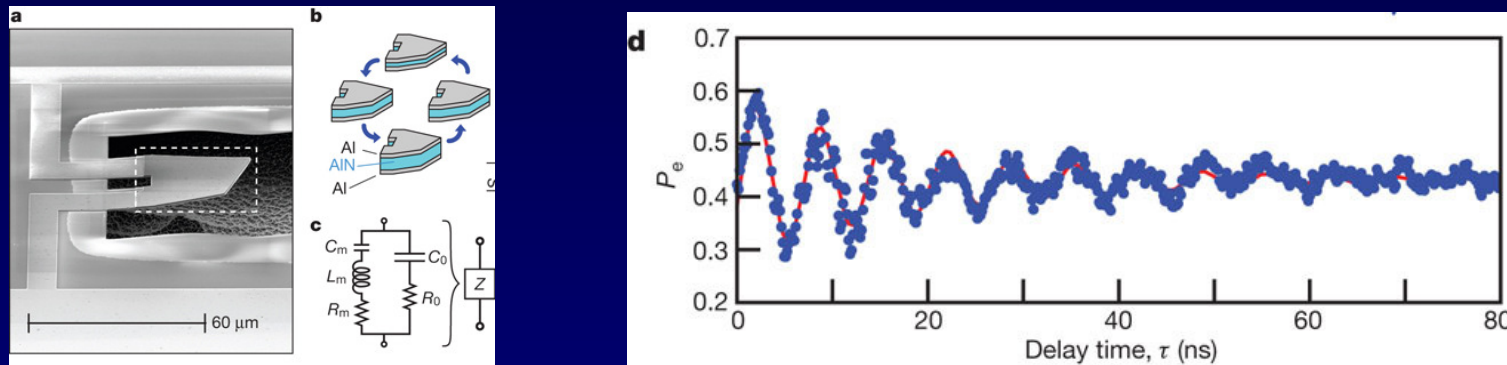
In any event, the correlations to the rest of the system cause *decoherence* and the *appearance of “collapse”*.

\*More correctly, we, the atom, and the cat become “entangled”.



# FYI: Recent Physics Milestone!

There has been a race over the past ~20 years to put a ~macroscopic object into a quantum superposition. The first step is getting the object into the ground state, below all thermal excitations. This was achieved for the first time in 2010, using vibrations in a small “drum” :



**“Quantum ground state and single-phonon control of a mechanical resonator”,**  
A. D. O’Connell, et al., *Nature* **464**, 697-703 (1 April 2010)

Quantum mechanics provides a highly accurate description of a wide variety of physical systems. However, a demonstration that quantum mechanics applies equally to macroscopic mechanical systems has been a long-standing challenge... Here, using conventional cryogenic refrigeration, we show that **we can cool a mechanical mode to its quantum ground state** by using a microwave-frequency mechanical oscillator—a ‘quantum drum’... We further show that **we can controllably create single quantum excitations (phonons) in the resonator**, thus taking the first steps to complete quantum control of a mechanical system.

# Entanglement

If we have two quantum systems, there are two possibilities for the total quantum state:

1. can be written as a product of the two individual systems:

$$\psi_{total} = \psi_1 \psi_2$$

2. cannot be written as a product:

$$\psi_{total} \neq \psi_1 \psi_2$$

We've seen several examples before in this course:

Atom that just emitted a photon:

$$\psi_{total} = \int d\vec{k} \psi_{atom}(\vec{k}) \psi_{photon}(-\vec{k})$$

Photon emitted in all directions; atom must recoil in opposite direction.

S. cat:  $\psi_{total} = \psi_{atom}(\textit{excited}) \psi_{cyanide\ vial}(\textit{"unbroken"}) \psi_{cat}(\textit{"alive"}) + \psi_{atom}(\textit{decayed}) \psi_{cyanide\ vial}(\textit{"broken"}) \psi_{cat}(\textit{"dead"})$

Double slit with quantum which-path detector:

$$\psi_{total} = \psi_{photon}(\textit{"upper slit"}) \psi_{detector\ 1}(\textit{"yes"}) \psi_{detector\ 2}(\textit{"no"}) + \psi_{photon}(\textit{"lower slit"}) \psi_{detector\ 1}(\textit{"no"}) \psi_{detector\ 2}(\textit{"yes"})$$

# Lasers

Photons are emitted when the electrons in atoms go from a higher state to a lower state

Conversely, photons are absorbed when the electrons in atoms go from a lower state to a higher state



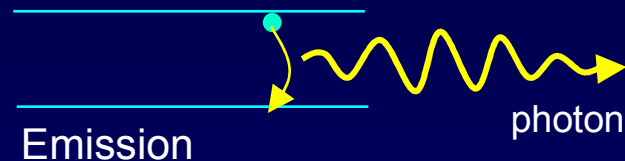
Fermions and bosons:

Electrons, protons, and neutrons are fermions. Two identical fermions cannot occupy the same quantum state. (exclusion principle)

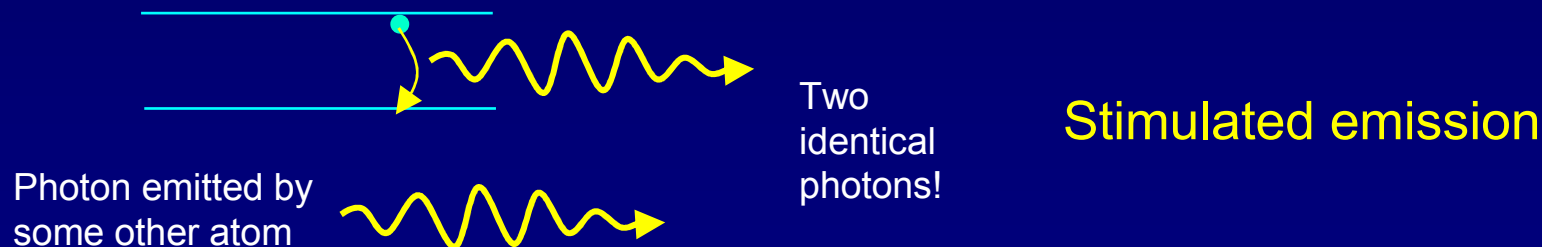
Photons (and many atoms) are bosons. Unlike fermions, bosons actually “prefer” (to be explained soon) to be in the same quantum state. This is the physical principle on which lasers are based.

# Lasers

Suppose we have an atom in an excited state. Eventually (at some random time) it will emit a photon and fall to the lower state. The emitted photon will go in a random direction. This is called “spontaneous emission”.



Suppose, however, that before the spontaneous emission occurs, another photon of the same energy (emitted by another atom) comes by. Its presence will stimulate the atom to emit its photon.



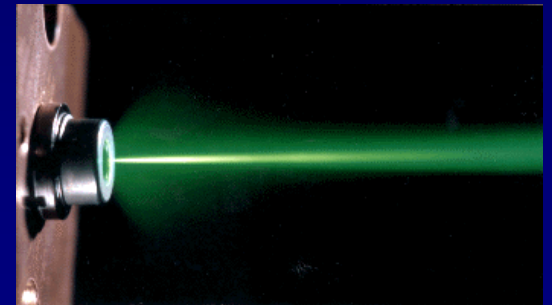
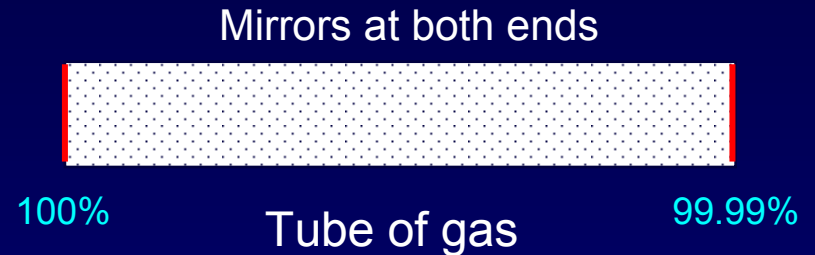
We now have two photons in the same quantum state: the same frequency, the same direction, and the same polarization. As they travel, they will stimulate even more emission.

# Lasers

## Light Amplification by Stimulated Emission of Radiation

### Laser operation (one kind):

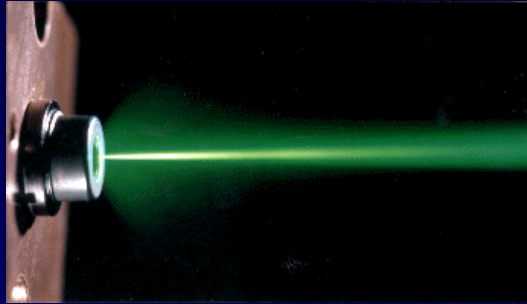
- Tube of gas with mirrored ends.
- Excite the atoms to the upper state (mechanism not shown).
- Spontaneous emission generates some photons.
- Photons that travel along the axis are reflected. Other directions leak out the sides.
- Because the amplification process is exponential, the axial beam quickly dominates the intensity.
- One mirror allows a small fraction of the beam out.



# Lasers

LASER:

“Light Amplification by Stimulated Emission of Radiation”



What if you don't have an atom that emits the color you want?  
“Make” one (e.g., by stressing the crystal lattice).

Did you know:

Semiconductors don't naturally emit in the red. Charles Henry (UIUC '65) discovered how to combine layers of different semiconductors to make a 'quantum well' (essentially a 1-D 'box' for electrons). By adjusting the materials, one could shift the emission wavelengths into the visible. Nick Holonyak (UIUC ECE Prof) used this to create the first visible LEDs & visible laser diodes.

# Magnetic Moments of Atoms

Electrons have a magnetic moment. Consequently, many atoms (e.g., iron) do as well. However, atoms that have completely filled orbitals never have a magnetic moment (in isolation). Why is this?

# Solution

Electrons have a magnetic moment. Consequently, many atoms (e.g., iron) do as well. However, atoms that have completely filled orbitals never have a magnetic moment (in isolation). Why is this?

An orbital is a set of states, all with the same  $(n, \ell)$ .

There are  $2\ell+1$   $m_\ell$  values and 2  $m_s$  values.

When the orbital is completely full, the angular momentum of the electrons sums to zero, because for every positive value of  $m_\ell$  and  $m_s$ , there is a corresponding negative one.

Therefore, there cannot be any magnetic moment (which results from “orbiting” charge).



# Noble (Inert) Gases

Except for helium, the electronic configuration of all the noble gases has a just-filled p orbital. What is the atomic number of the third noble gas (neon is number 2)?

# Solution

Except for helium, the electronic configuration of all the noble gases has a just-filled p orbital. What is the atomic number of the third noble gas (neon is number 2)?

This is just a counting problem:

$$2 + 2 + 6 + 2 + 6 = 18 \text{ That's argon.}$$

$$1s \quad 2s \quad 2p \quad 3s \quad 3p$$

neon



Periodic Table of the Elements

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

* Lanthanide Series	58	59	60	61	62	63	64	65	66	67	68	69	70	71
	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
+ Actinide Series	90	91	92	93	94	95	96	97	98	99	100	101	102	103
	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

# Another Inert Gas Question

Why is it that (except for helium) the electronic configuration of all the noble gases has a just-filled p orbital? Can we understand helium also?

# Solution

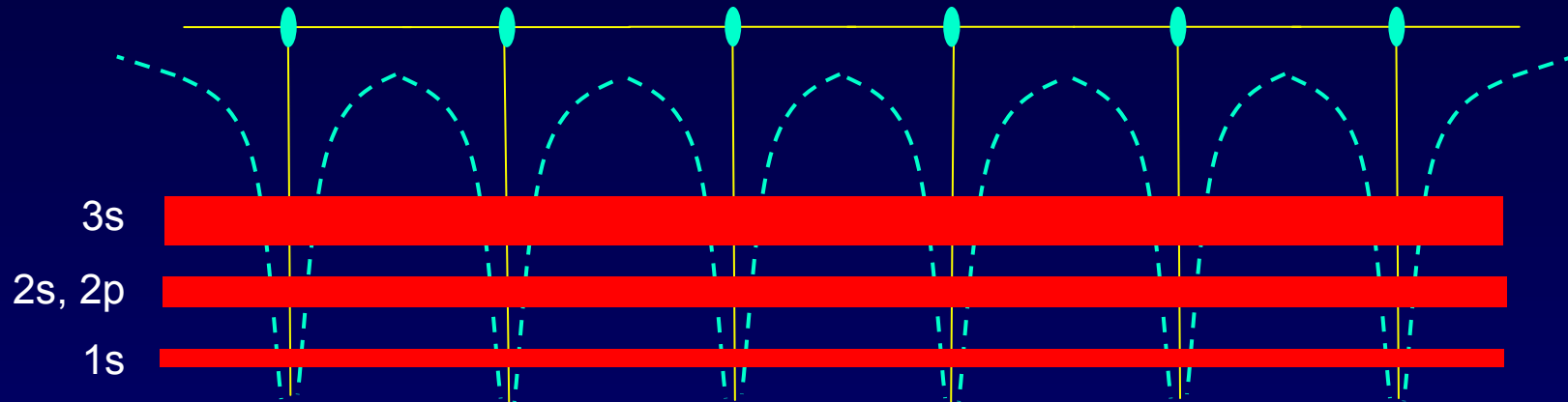
Why is it that (except for helium) the electronic configuration of all the noble gases has a just-filled p orbital? Can we understand helium also?



Look at the order in which the states are filled. The atom just after each noble gas (including helium!) is the first to have an electron in the next n-shell. For example, sodium follows neon and is the first atom to have an electron in an n=3 state. The big energy gap makes it difficult for the noble gas electrons to form chemical bonds.

# Band Widths

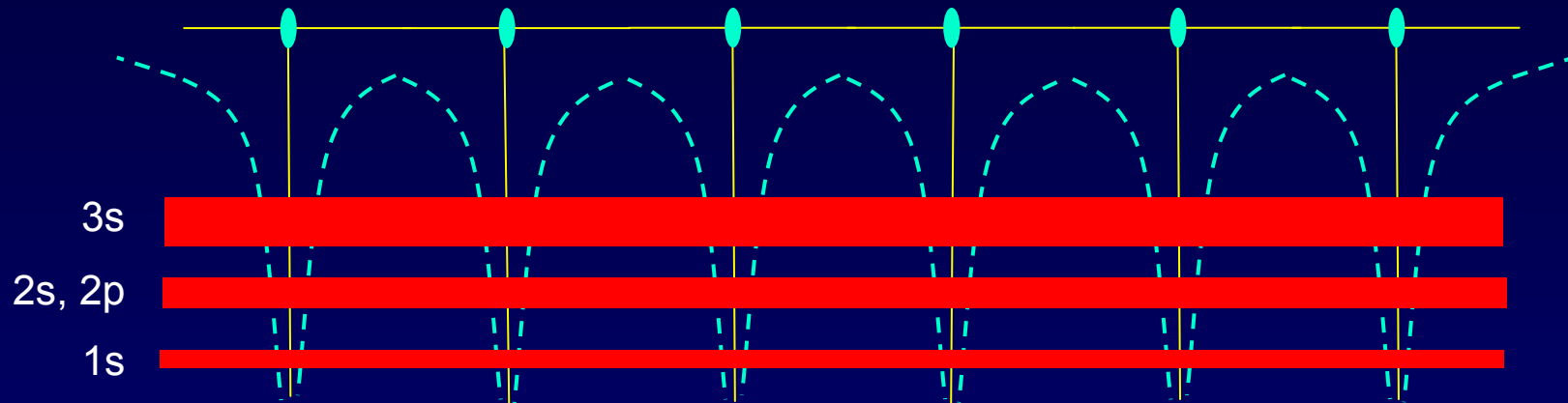
Why is the 3s band wider (bigger energy spread) than 1s, 2s, or 2p?



- a. Because  $n$  is larger.
- b. Because it overlaps with the 3p band (not shown).
- c. Because  $E_{3s}$  is larger.

# Solution

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- a. Because  $n$  is larger.
- b. Because it overlaps with the 3p band (not shown).
- c. Because  $E_{3s}$  is larger.

- a) You might think this is equivalent to c), but beware. For larger  $n$  values, the order can be reversed. 6s has lower energy than 5p.
- b) may be true, but the presence of the 3p band does not affect 3s energy levels.
- c) Higher energy means that there is more tunneling. This causes the symmetric wave functions to have a larger energy shift.

THE END

Best wishes in Physics 213  
and  
all your other courses!