# Wed. Oct. 31



- We now have sufficient background to investigate one of the most important topics in solid state physics

- "Band theory" or "electronic band structure" describes the allowed energy values within solids → that is the electrons making up the solid

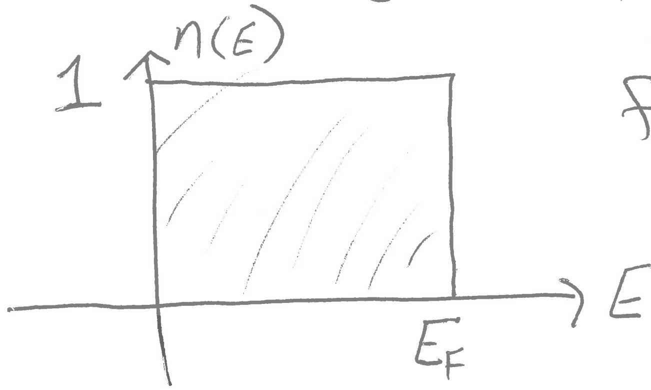
- Just as atoms & molecules have allowed energy levels for their electrons, solids, which are essentially large molecules, show the same behavior

- Solids instead have quasi-continuous bands of energy values

- Our first encounter with electrons in solids involved the free "electron model," in which the electrons were modelled as a charged gas bound by boundaries of the solid

→

- inside the solid, the electrons experienced no potential but external EM fields
- due to the Pauli exclusion principle, the valence electrons in a conductor have energies within a band $0 < E \leq E_F$, where $E_F$ is the Fermi energy (for $T=0$)
- the probability $n(E)$ that an electron energy is occupied is given by Fermi-Dirac stats:




for $T=0$

- despite many successes this model had for describing conductors, we know some solids have forbidden energies, call "band gaps"
- since we ignored electron/lattice interactions for the free electron, a possible place to look for the cause of band gaps is this interaction

- We guess that the principles of diffraction we just developed extends to electron transport within solids

- this should be true since electrons have wavelike properties, a quantum effect

- let's recall what QM tells us about atoms

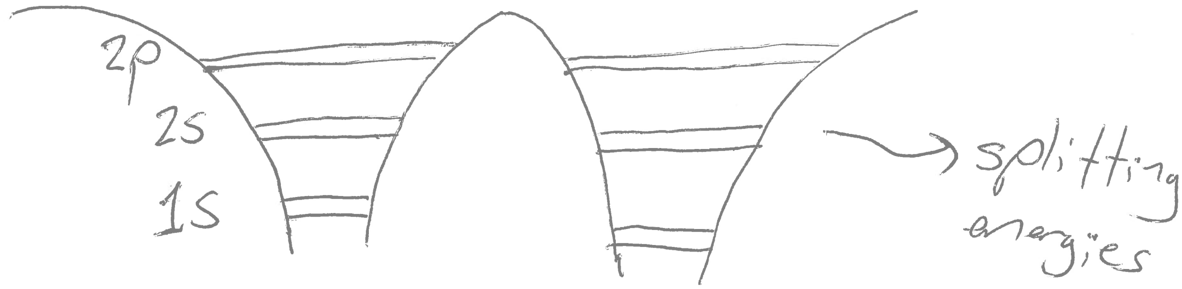
- we solve the Schrödinger equation for electrons in a potential well (interaction with positive nucleus) + we obtain discrete energy values for electron orbitals

- As a qualitative example, a Li atom
  - → completely full 1s shell (↑ + ↓ spins)
  - → one $e^-$ in the 2s subshell
  - → 2p first excited state


lines are discrete energies

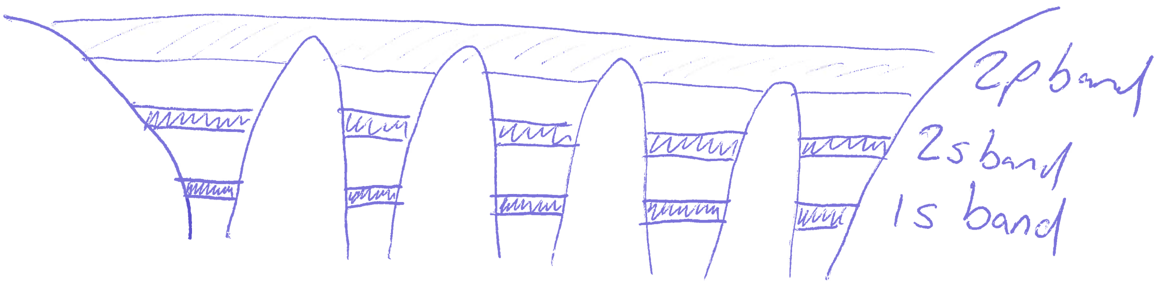
$V(\vec{r})$ for a single atom of Li

- Now let's form a $Li_2$ molecule:

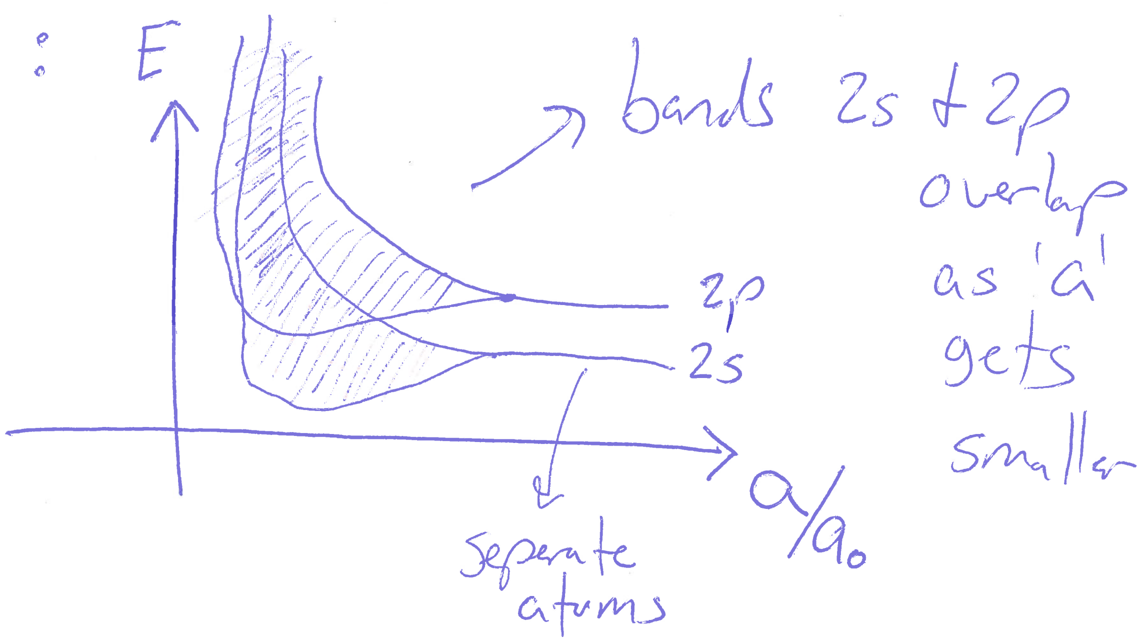



- We find that the presence of the second nucleus splits the energy levels, represented by horizontal lines
- each molecular level can accomodate 2 electrons (spin ↑ + ↓)
- For $Li_2$, 4 electrons are in 1s orbitals + 2 in the 2s subshell
- the splitting is actually larger for higher energy states → electrons "screen" nuclei

- for a solid made of lithium atoms (cluster)

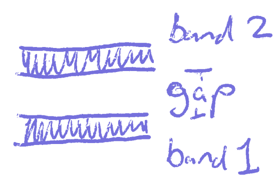



- What we find for large #'s of atoms, the bands become wider & overlap
- where they overlap depends upon their interatomic spacing, 'a'
- roughly :




$a_0 \rightarrow$ atomic radius (approximately)

- this idea of energy levels splitting into bands is arguably the most important discovery in solid state physics




- the consequent idea of "band gaps" is the foundation of semiconductor physics, making possible modern electronics

- to see impact, industry started ~1960 & in 2017 was valued at ~\$412,000,000,000

- very roughly, conductors have overlapping bands (no gaps), semiconductors have narrow gaps, and insulators have wide gaps (electron energy levels within solids)

- Example: titanium dioxide in anatase crystal phase has a band gap of ~3.2eV which corresponds to $\lambda \sim 390nm$. When UV photon with energy higher than ~3.2 eV, an electron can be promoted to the conduction band, so $TiO_2$ becomes a conductor & a catalyst.
  → we will hopefully have time to discuss later

- we have a semi-qualitative description of bands in solids
- let's make it a bit more qualitative
- recall the energy of an electron for the free electron model $\propto k^2$

$$E_k = \frac{\hbar^2 k^2}{2m}, \quad k = \pm 2\pi n / L, \quad L \equiv \text{length of solid}$$

- our solution is a travelling wave (1D)

$$\psi_k(x) = \frac{e^{ikx}}{\sqrt{L}}$$

- just as we found for phonons, travelling vibrational quantized energy packets, the electrons also get diffracted by the lattice
- we first consider the dispersion relation for the "empty lattice" so just the free electron model again

- for 1D case, we know the k-axis is periodic

$$k + G = k$$

where G is the reciprocal lattice point (vector in 3D)