30 — picking up from previous — we have a homogeneous model of a solid with electrons moving freely. we've turned off interactions between electrons.

If we use "hard" boundary conditions ($\psi = 0$ at the edge of the crystal) then wave function is:

$$\psi = \sqrt{\frac{8}{\ell_x \ell_y \ell_z}} \sin\Big(\underbrace{\frac{\pi}{\ell_x} n_x}_{k_x} x\Big) \sin\Big(\underbrace{\frac{\pi}{\ell_y} n_y}_{k_y} y\Big) \sin\Big(\underbrace{\frac{\pi n_z}{\ell_z}}_{k_z} z\Big)$$

$$E = \frac{\hbar^2 k^2}{2m} \qquad \vec{k} = (k_x, k_y, k_z) \leftarrow \text{vector}$$

Remark repeated: we'd be better off using a wavefunction $\psi = e^{i\vec{k}\cdot\vec{r}}$ with periodic boundary conditions:

$\psi(x, y, z) = \psi(x + \ell_x, y, z)$ — thats what you will do next semester in Stat Mech

$$\vec{k} = \frac{\pi}{L}\overbrace{(n_x, n_y, n_z)}^{\vec{n}\text{ vector}}$$

Energy level diagram in simple case $\ell_x = \ell_y = \ell_z$

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 \pi^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2)$$

— — — — — — (3,2,1)

— — — (3,1,1)

— — — (2,2,1)

— — — (2,1,1)

— (1,1,1)

If we have to put 6×10^{23} arrows in this diagram as we did for atoms its going to take a lot of time!

Alt: the $\vec{k} = \left(\frac{\pi}{\ell_x} n_x, \frac{\pi}{\ell_y} n_y, \frac{\pi}{\ell_z} n_z\right)$ for all possible values of n_i form a lattice in $\vec{k}$ space — every state [(n_x, n_y, n_z) choice] can be thought of as the end of a k brick

If we seek the low energy states - these will be nearest the $\vec{k}$ origin. If we have N electrons we need $\frac{N}{2}$ bricks (states) each as close to the origin as possible — since the electrons are fermions once a brick has been layed (ie a state populated) that spot is filled — no additional brick can be placed there.

So given N electrons and therefore $\frac{N}{2}$ bricks we want to place those bricks as close to the origin as possible to get the lowest energy state — that is we want to make a Lego version of a sphere.

A sphere (actually $\frac{1}{8}$ sphere since $n_i \geq 0$) will hold:

radius of sphere in k-space
F = Fermi

$$\frac{\frac{1}{8}\,\frac{4}{3}\,\pi\, k_F^3}{\frac{\pi}{l_x}\,\frac{\pi}{l_y}\,\frac{\pi}{l_z}} = \frac{N}{2}$$

size of a brick

electrons

2 electrons per state: ↑↓

$$\frac{1}{3\pi^2} k_F^3 = N/V$$ } number density : n

The energy of the last filled state ("Fermi Energy")

$$E_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m}\left(3\pi^2 n\right)^{2/3}$$

$$\text{The average energy} = \frac{\frac{\hbar^2}{2m}\int_0^{k_F} k^2\, \frac{1}{8} 4\pi k^2\, dk}{\int_0^{k_F} \frac{1}{8}4\pi\, k^2\, dk} = \frac{\frac{\hbar^2}{2m}\,\frac{1}{5}k_F^5}{\frac{1}{3}k_F^3}$$

$\langle E \rangle$

$$= \frac{3}{10}\,\frac{\hbar^2 k_F^2}{\cancel{2}m}$$

$$\text{total energy} = \langle E \rangle N = \frac{3}{10}\,\frac{\hbar^2 k_F^2}{\cancel{2}m}\,\overbrace{\frac{1}{3\pi^2} k_F^3\, V}^{N}$$

$$= \frac{3}{10}\,\frac{\hbar^2}{\cancel{2}m}\left(3\pi^2 \frac{N}{V}\right)^{2/3} N = \frac{\hbar^2\left(3\pi^2 N\right)^{5/3}}{10\pi^2\, m}\, V^{-2/3}$$

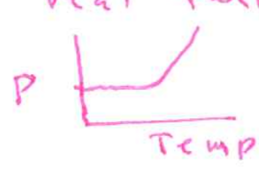
One can show the pressure $= P = \frac{2}{3}\frac{E_{tot}}{V} = \frac{(3\pi^2)^{2/3}\hbar^2}{5\, m}\, n^{5/3}$

(Remark: this is for nonrelativistic particles)

In 211 you learned the ideal gas law: $P = nkT$

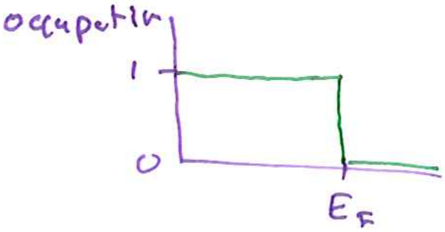
The above calculation applies to an electron gas where all the energy possible was removed — ground state at $T=0$

evidently, unlike ideal gas, a real fermion gas has a pressure even at $T=0$

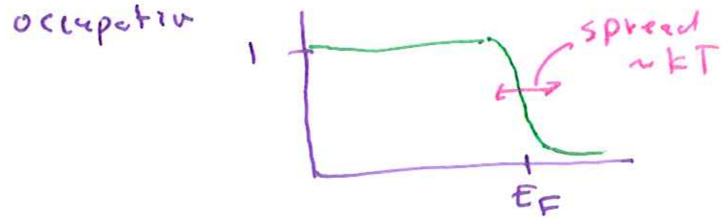


"degeneracy pressure"

In filling the states of our electron gas we always put the next electron in the lowest available (unfilled) state. If we plot the "occupation number" vs energy of state it would look like a sharp cut-off



If at a non zero temp some electrons will gain a bit of thermal energy



Consequences:

- In a normal gas if you increase the temperature every atom gets a bit more energy: $\langle KE \rangle = \frac{3}{2} kT$
  In this degenerate electron gas the only electrons that can change (increase) energy are those near the "surface" — reduced specific heat results
- If electrons "try" to scatter most often (except for electrons near the "surface") the state they might try to go to will already be occupied — can't change directions as there are no available options. Result — long mean free path even thru dense gas

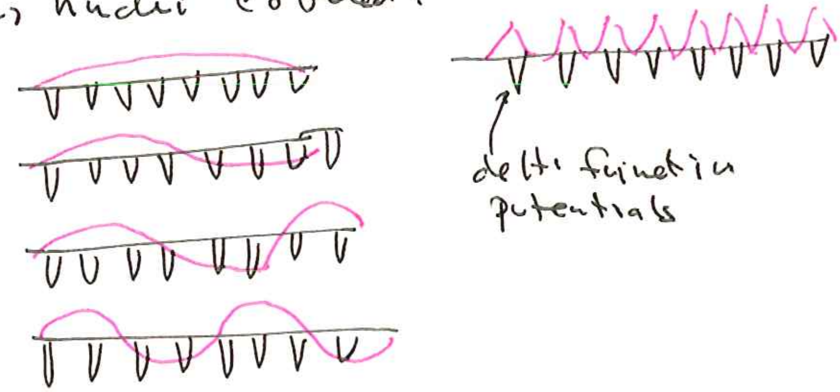
Bring back nuclei (kill translation invariant Jelly) but just in 1d. Consider N δ function potentials spaced by a

For N=2 & nuclei sufficiently far apart there are 2 bound states: symmetric & antisymmetric

If add more nuclei get more states with approx same E

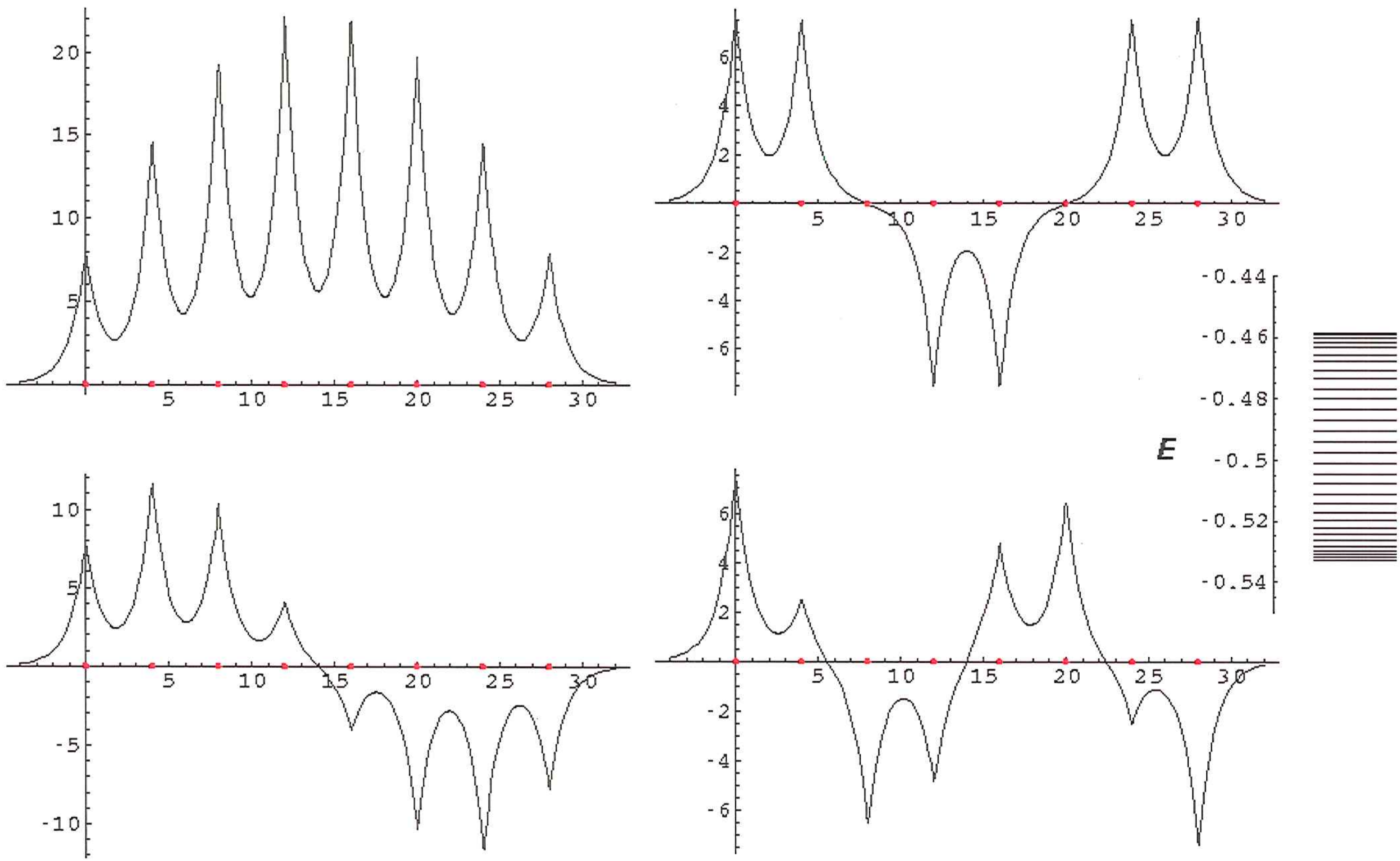
The states (see following page) seem to "want" to be a combination of every nuclei covered:

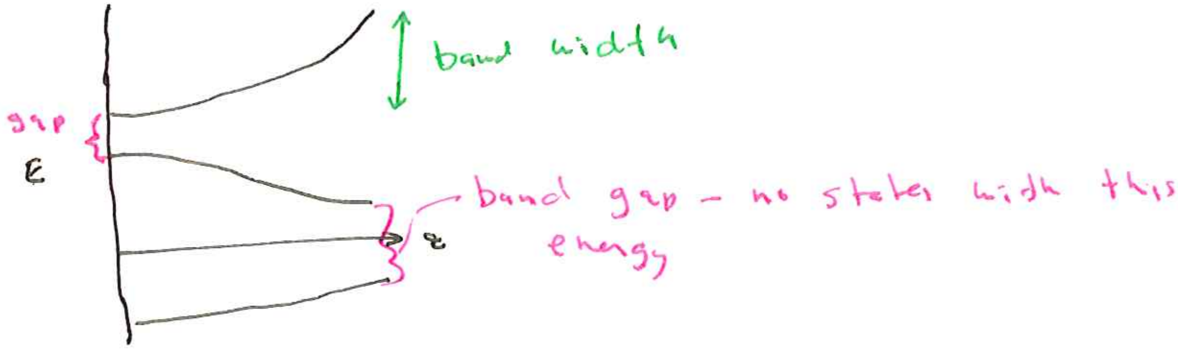
times a standing wave



the eigenenergies cluster together - but there seems to be an uneven "density of states"

These properties carry into the solution to an actual infinite N. With an actually infinite N comes an actually infinite number of states indexed by a real number q. $q=0$ is going to make symmetric combo of states, small q makes a long wavelength of variation; largest q makes alternating phases.


E
-0.44
-0.46
-0.48
-0.5
-0.52
-0.54



Using the usual time dependent QM we show that if at $t=0$ ψ is concentrated on one nucleus, over time it moves on — narrow bands have slow "hopping" rate wider bands faster.

For any q there is a wave function (actually several in other bands) that covers the universe – these states need to be filled with (at this point) non interacting electrons. [It might be easier to think about quantizing q with a large finite # of nuclei & hence a large but not infinite # of electrons to be placed]

The mathematical details fall under the names Bloch's Thm or Floquet's Thm – $\psi(x)$ is written in terms of an actually periodic function $u_q(x)$ and a wave: $e^{iqx} \rightarrow \psi(x) = e^{iqx} u_q(x)$

For any fixed value of q, solve Schrodingers Eq. $\Rightarrow E(q)$. Finally note that q has a bounded range called a Brillouin Zone