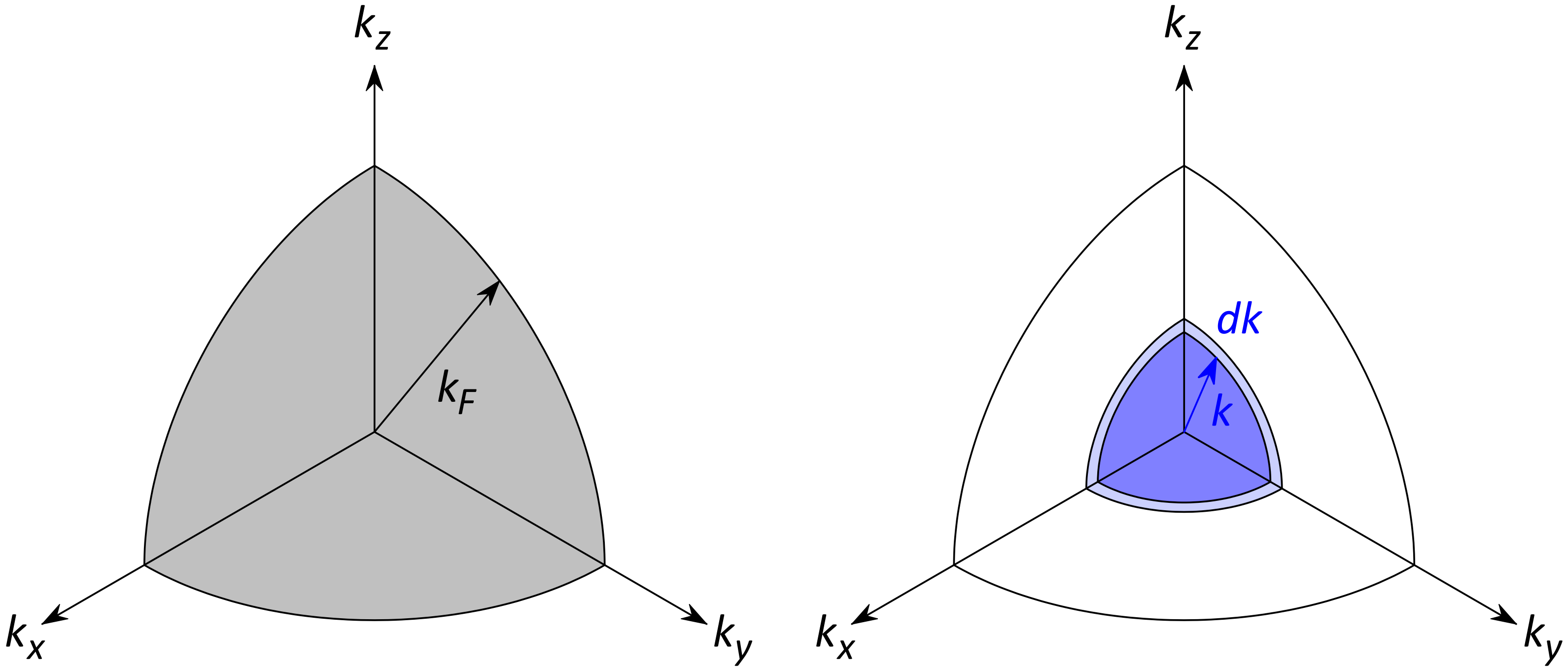
Today in Physics 237: k space

- Free electrons in a rectangular box, or equivalently an octant in *k* space.
- Total energy of a Fermi gas.
- Degeneracy pressure



Free electron gas in a box

- Imagine a solid object to be rectangular, with dimensions $\ell_x, \ell_y,$ and ℓ_z.

- And suppose the nuclei of the constituent atoms are fixed in position, but that the electrons are **free** to move within the solid, with no forces on them. Then the time-independent Schrödinger equation separates into three:

$$-\frac{\hbar^2}{2m_e}\nabla^2\psi = E\psi \quad \Rightarrow \quad -\frac{\hbar^2}{2m_e}\frac{d^2X}{dx^2} = E_x X \quad , \quad -\frac{\hbar^2}{2m_e}\frac{d^2Y}{dy^2} = E_y Y \quad , \quad -\frac{\hbar^2}{2m_e}\frac{d^2Z}{dz^2} = E_y Y \quad .$$

- This is an N-quantum state – we have $N \ggg\gg 1$ in mind – in a 3-D rectangular box; constraining each electron to the box makes it easier to use sines and cosines in the free-quantum solution rather than complex exponentials:

$$X(x) = A_x \sin k_x x + B_x \cos k_x x \quad , \quad k_x = \frac{\sqrt{2m_e E_x}}{\hbar} = \frac{n_x \pi}{\ell_x} \quad n_x = 0,1,2,\ldots$$

and similarly for y and z. Put the origin at the center of the box. As in the original quantum-in-a-box (Lecture 8), the vanishing of the wavefunction at the walls makes all the Bs zero, and normalization over the volume adds three factors of $\sqrt{2}$:

Free electron gas in a box (continued)

$$\psi_{n_x n_y n_z} = \sqrt{\frac{8}{\ell_x \ell_y \ell_z}} \sin\left(\frac{n_x \pi}{\ell_x} x\right) \sin\left(\frac{n_y \pi}{\ell_y} y\right) \sin\left(\frac{n_z \pi}{\ell_z} z\right) \quad ,$$

with $$E_{n_x n_y n_z} = \frac{\hbar^2}{2m_e}\left[\left(\frac{n_x}{\ell_x}\right)^2 + \left(\frac{n_y}{\ell_y}\right)^2 + \left(\frac{n_z}{\ell_z}\right)^2\right] \equiv \frac{\hbar^2}{2m_e}\left(k_x^2 + k_y^2 + k_z^2\right) \equiv \frac{\hbar^2 k^2}{2m_e} \quad .$$

- Here k is as usual the magnitude of the wavevector $\boldsymbol{k} = \boldsymbol{p}/\hbar$.
- Now imagine expressing all this in the three-dimensional space of wavevector components $\begin{bmatrix} k_x & k_y & k_z \end{bmatrix}$, which we call ***k* space**:
  - Each point in k space corresponds to a distinct single-quantum state with distinct values of $\begin{bmatrix} k_x & k_y & k_z \end{bmatrix}$.
  - And each single quantum state may be said to occupy a ***k*-space** volume $\frac{\pi}{\ell_x}\frac{\pi}{\ell_y}\frac{\pi}{\ell_z} = \frac{\pi^3}{V}$.

Free electron gas in a box (continued)

- So far this is nothing more than the *N* quantum version of the free wavepacket:
  - Instead of referring to a quantum's position-basis wavefunction ψ and location $\boldsymbol{r}$ we could refer to its momentum-basis wave function φ and momentum $\boldsymbol{p} = \hbar \boldsymbol{k}$.
  - This effectively moves us to Fourier-transform space (cf. Lecture 7).
- If electrons were identical bosons, and we were to continue to ignore electrostatic repulsion and kinetic energy of thermal origin, the exchange force would collect all the quanta into one state.
  - Semiconductor physics would be much less interesting in this case. (Not superconductor physics, though.)
- Electrons are identical fermions, though, so the exchange force – agent of the Pauli principle – distributes their points in *k* space **uniformly**, with **two** allowed per *k*: spin up and spin down.
  - If there are *N* atoms in the box, and each contributes *d* free electrons, then the electrons take up a *k*-space volume $V_k = (Nd/2)\left(\pi^3/V\right)$.

Free electron gas in a box (continued)

- Given that k is a positive real number, and supposing that the rectangular volume V is cubical, then all the $Nd/2$ points occupy an octant of a sphere in k space, which has radius k_F given by

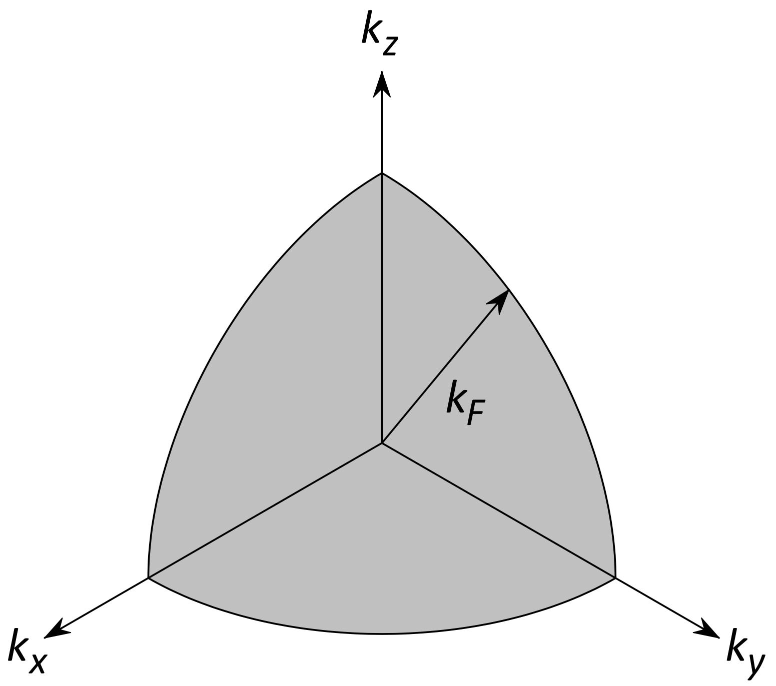
$$\frac{1}{8}\left(\frac{4\pi}{3}k_F^3\right)=\frac{Nd}{2}\left(\frac{\pi^3}{V}\right) \Rightarrow k_F^3=3\left(\frac{Nd}{V}\right)\pi^2 \Rightarrow k_F=\left(3\rho\pi^2\right)^{1/3} ,$$

where $\rho=Nd/V$ is the **number** density of free electrons.

- The surface of the octant, **separating occupied and unoccupied states**, is called the **Fermi surface**.
  - Its radius and the corresponding energy

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

are also named after Fermi.



Warning: in astrophysics classes like ASTR 142, $Nd/2$ would be given the symbol n, with $\rho=mn$ $(m_e n$ in this case$)$.

Free electron gas in a box (continued)

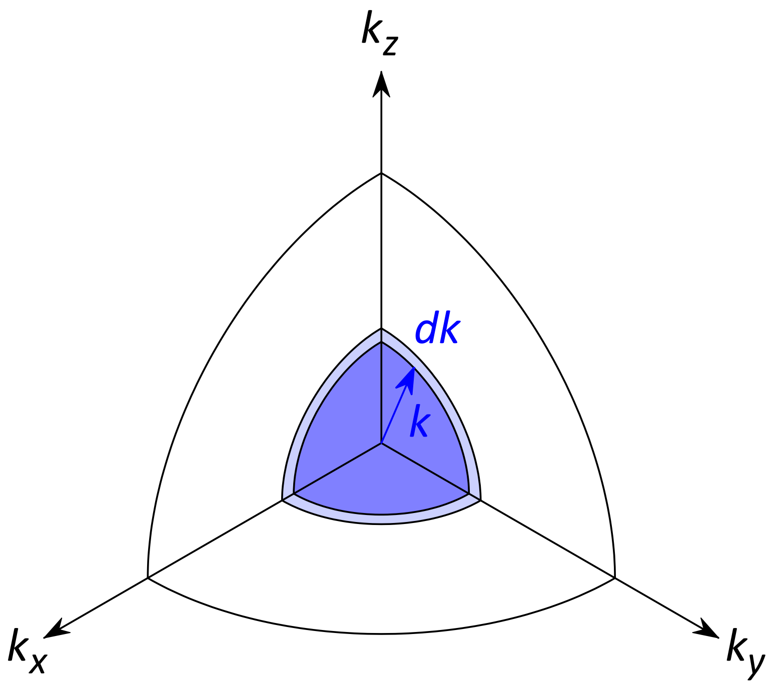
- From here we can calculate the total energy of the electron gas. Take an infinitesimal shell of the octant, with volume

$$dV_k = \frac{1}{8}\left(4\pi k^2 dk\right).$$

- The number of electron states contained there is

$$dn = Nd\frac{dV_k}{\frac{Nd}{2}\left(\frac{\pi^3}{V}\right)} = \frac{\frac{1}{2}\pi k^2 dk}{\frac{1}{2}\left(\frac{\pi^3}{V}\right)} = \frac{V}{\pi^2}k^2 dk$$

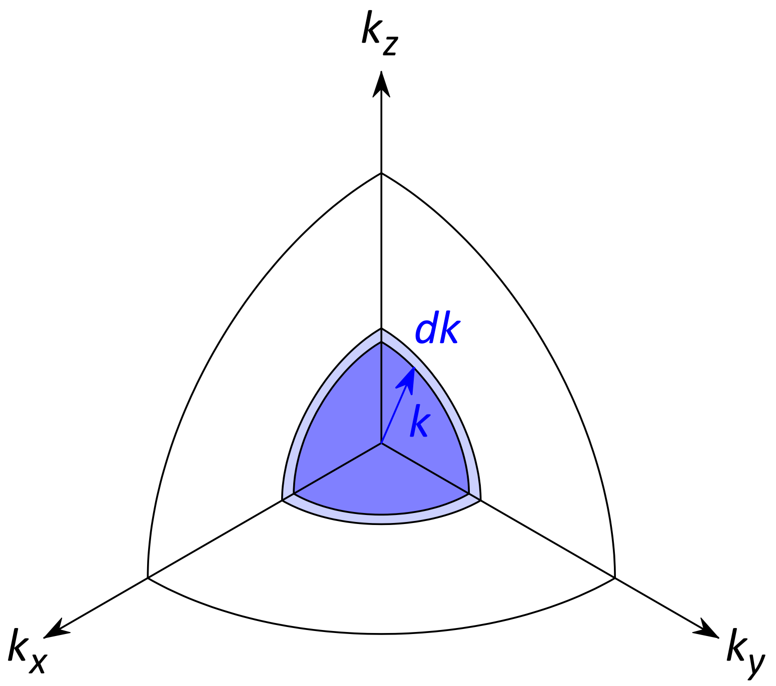
- Each state has energy $\frac{\hbar^2 k^2}{2m_e}$, so we integrate:



Free electron gas in a box (continued)

$$E_{\text{total}} = \frac{\hbar^2 V}{2\pi^2 m_e}\int_0^{k_F} k^4 dk = \frac{\hbar^2 V k_F^5}{10\pi^2 m_e} = \frac{\hbar^2 V}{10\pi^2 m_e}\left(3\left(\frac{Nd}{V}\right)\pi^2\right)^{5/3}$$

$$= \boxed{\frac{\hbar^2\left(3\pi^2 Nd\right)^{5/3}}{10\pi^2 m_e}V^{-2/3}}\,.$$



- Note that the total energy decreases as volume increases.

Degeneracy pressure

- Now imagine changing the volume of the box, for the same contents, by a small amount. This takes a small amount of work:

$$dW = \frac{dE_{\text{total}}}{dV}dV = -\frac{2}{3}\frac{\hbar^2\left(3\pi^2 Nd\right)^{5/3}}{10\pi^2 m_e}V^{-5/3}dV = -\frac{2}{3}E_{\text{total}}\frac{dV}{V} \quad .$$

- If we view the Pauli exclusion principle to work by the agency of the exchange force, it is that force – or, more precisely, the geometry of the states enforced by antisymmetry – which does the work.

- For a pressure P which does work against its surroundings, $dW = -PdV$, so we can write the expression above as a pressure:

$$P_{\text{d}} = \frac{2}{3}\frac{E_{\text{total}}}{V} = \frac{2}{3}\frac{\hbar^2\left(3\pi^2 Nd\right)^{5/3}}{10\pi^2 m_e}V^{-5/3} = \boxed{\frac{\hbar^2\left(3\pi^2\right)^{2/3}}{5m_e}\rho^{-5/3}}$$

Degeneracy pressure

Compare to ASTR 142, in which we get $P_d = 2\pi^2\hbar^2\rho^{-5/3}/m_e$.