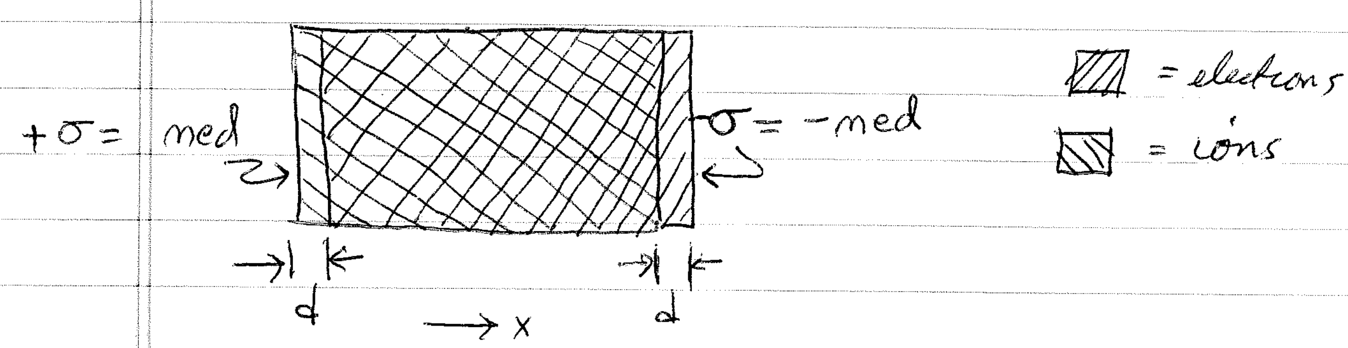
Plasmon

Although we argued by screening that e-e interactions are less important than one might naively expect, nevertheless the Coulomb interaction between electrons does give rise to physically interesting effects.

One such effect is the plasmon - which is a longitudinal charge density oscillation.

Simple explanation: consider the gas of electrons as a rigid charged body of mass $mN = mnV$ where N is the total number of electrons. If we displace the electrons a distance d with respect to the ions, we will create a surface charge on the surfaces of the system as shown below.



Surface charge σ creates electric field inside

$$\vec{E} = 4\pi\sigma\hat{x} = 4\pi ned\,\hat{x}$$

Newton's equation of motion for the electrons is then

$$mN\ddot{d} = -eNE = -4\pi ne^2 d N$$

$$\ddot{d} = -\frac{4\pi ne^2}{m} d$$

$\rightarrow$ harmonic oscillation at frequency $\boxed{\omega_p = \sqrt{\frac{4\pi ne^2}{m}}}$

the plasma frequency!

$\Rightarrow$ oscillation in charge and $\vec{E}$ with freq ω_p.

<u>Another way to get plasma oscillations</u> from Maxwell's equations

When we considered EM wave propagation in a metal early in the course, we limited discussion to <u>transverse</u> modes where $\vec{k}\cdot\vec{E}=0$. The plasma oscillation is a <u>longitudinal</u> mode $\vec{k}\cdot\vec{E}\neq 0$.

charge conservation: $\vec{\nabla}\cdot\vec{j} = -\frac{\partial \rho}{\partial t}$

for harmonic oscillation: $\vec{j} = \vec{j}_0 e^{-i\omega t} e^{i\vec{k}\cdot\vec{r}}$

freq ω, wavevector $\vec{k}$ $\quad \rho = \rho_0 e^{-i\omega t} e^{i\vec{k}\cdot\vec{r}}$

$$\Rightarrow i\vec{k}\cdot\vec{j}_0 = i\omega\rho_0$$

But we also had $\vec{j}_0 = \sigma(\omega)\vec{E}_0 \qquad \sigma$ is ac conductivity

$$\Rightarrow i\vec{k}\cdot\sigma\vec{E}_0 = i\omega\rho_0$$

From Gauss's Law $\vec{\nabla}\cdot\vec{E} = 4\pi\rho$

$$\Rightarrow \quad i\vec{k}\cdot\vec{E}_0 = 4\pi\rho$$

Combine above with charge conservation to get

$$\frac{\sigma}{\omega}\vec{k}\cdot\vec{E}_0 = \frac{i\vec{k}\cdot\vec{E}_0}{4\pi}$$

~~Ithe~~ If there is to be a solution, then either

$$\vec{k}\cdot\vec{E}_0 = 0 \quad \Rightarrow \quad \text{transverse mode}$$

or

$$\frac{4\pi\sigma}{i\omega} = 1$$

$$\Rightarrow \quad \boxed{1 + \frac{4\pi i\sigma}{\omega} = 0}$$

We saw the above quantity earlier in our discussion of transverse wave propagation in metals. Then we had for the dispersion relation for the transverse EM waves:

$$k^2 = \frac{\omega^2}{c^2}\left[1 + \frac{4\pi i\sigma}{\omega}\right]$$

In analogy with dielectrics, one sometimes ~~writes~~ defines

$$\varepsilon(\omega) = 1 + \frac{4\pi i\sigma(\omega)}{\omega} \quad \text{for a metal}$$

$\uparrow$

complex ~~dielectr~~ frequency dependent dielectric function

Longitudinal
~~Plasma~~ oscillations occur when

$$\varepsilon(\omega) = 1 + \frac{4\pi i \sigma(\omega)}{\omega} = 0$$

From our discussion of the Drude model we had

$$\sigma(\omega) = \frac{\sigma_{dc}}{1 - i\omega\tau} \qquad \sigma_{dc} = \frac{ne^2\tau}{m}$$

For high frequencies $\underline{\underline{\omega\tau \gg 1}}$, $\sigma(\omega) \simeq \frac{\sigma_0}{-i\omega\tau}$

$$= \frac{ne^2}{-i\omega m}$$

and so

$$\varepsilon(\omega) = 1 - \frac{4\pi ne^2}{m\omega^2}$$

$$= 1 - \left(\frac{\omega_p}{\omega}\right)^2 \quad \text{with} \quad \omega_p = \sqrt{\frac{4\pi ne^2}{m}}$$

So the condition $\varepsilon(\omega) = 0$ for longitudinal modes of oscillation

$$\Rightarrow \boxed{\omega = \omega_p} \quad \text{for } \cancel{\text{all}} \text{ any wavevectors } \vec{k}$$

Such longitudinal modes are called "plasma" oscillations since ~~they are accompanied~~ the longitudinal oscillations of the electric field ($\vec{k} \cdot \vec{E}_0 \neq 0$) are (by Gauss' law) accompanied of oscillations in electron charge density.

Note, the above Maxwell eqn arguement gives a plasma oscillation at $\omega = \omega_p$ for any longitudinal wave vector $\vec{k}$. In reality, the ~~plasma freque~~ frequency of plasma oscillations <u>does</u> depend on $\vec{k}$.

In our derivation of $\sigma(\omega)$ we assumed that the wavelength λ of the EM oscillations was macroscopically large, ie $\gg$ atomic lengths. This lead to a $\sigma(\omega)$ independent of wavevector $\vec{k}$. (ie we ignored spatial dependence of $\vec{E}$ on equation of motion of electron). When one does a better job, one finds that $\varepsilon = 1 + 4\pi i\sigma(\omega)/\omega$ should really have a dependence on $\vec{k}$ as well, that is important when k is of the order $1/a_0$, ie $\lambda \sim a_0$ atomic length scale. (Recall the k-dependence of the Thomas-Fermi dielectric function for the $\omega = 0$ case). If one includes this k dependence of $\varepsilon(\vec{k}, \omega)$, then the condition $\varepsilon(\vec{k}, \omega) = 0$ gives a dispersion relation for plasma oscillations:

$$\omega_p(\vec{k}) \simeq \omega_p \left[1 + \frac{3}{10} \frac{v_F^2 k^2}{\omega_p^2} \right]$$

where $\omega_p = \sqrt{4\pi n e^2/m}$ as before
and v_F is the Fermi velocity

Note $$\frac{v_F^2 k^2}{\omega_p^2} = 4 \left(\frac{\varepsilon_F}{\hbar\omega_p}\right)^2 \left(\frac{k}{k_F}\right)^2$$

For Typical metals, $\varepsilon_F \sim 2-10$ eV

$\hbar\omega_p \sim 10-20$ eV

$\Rightarrow$ correction to ω_p at finite k is usually quite small for $k < k_F$.

As with other harmonic oscillations, the longitudinal plasma oscillations of electrons in a metal, get quantized in a more complete quantum mechanical treatment of the EM fields. When so quantized, the plasma oscillations are refered to as "plasmons". ~~and have energy~~ The energy associated with the n^{th} level of excitation of the oscillations with wavevector $\vec{k}$, ie the energy of n plasmons of wave vector $\vec{k}$, is just $(n+1/2)\hbar\omega_p(\vec{k})$.

Because $\hbar\omega_p \sim 10-20$ eV $\gg k_BT$, plasmons are not in general thermally excited. However the zero point energy of the plasmon modes, ie the $\frac{1}{2}\hbar\omega_p(\vec{k})$, does contribute to the ~~ground state~~ total ground state energy of the electron gas.

When one shoots a high energy electron into a metal surface, one can see energy loses corresponding to the excitation of integer numbers of plasmons with energies $n\hbar\omega_p$.

Another moral from the story of the plasmon:

We start with electrons which are fermions.
A bare electron has energy $\varepsilon(k) = \frac{\hbar^2 k^2}{2m}$.

When we include effects of the Coulomb interactions among the electrons in a gas of electrons, we get not only fermionic degrees of freedom with dispersion relation $\varepsilon(\vec{k}) = \frac{\hbar^2 k^2}{2m}$, but now we also get bosonic degrees of freedom, ie the plasmons with dispersion relation

$$\hbar\omega_p(\vec{k}) \simeq \hbar\omega_p\left(1 + \frac{3}{10}\frac{v_F^2 k^2}{\omega_p^2}\right)$$

(goes to constant ω_p as $k \to 0$.
weak dependence on k for small $k < k_F$.

Moral: The presence of strong interactions among the "bare" (ie isolated) degrees of freedom can lead to elementary excitations (ie new degrees of freedom) of the system that bear no resemblance at all to the bare degrees of freedom – ie they can have a completely different dispersion relation $\varepsilon(\vec{k})$ and can even have different symmetry, ie bosonic instead of fermionic. This is a general rule to remember in all fields of physics! (Another condensed matter example is phonons: bare ions have $\varepsilon(k) = \frac{\hbar^2 k^2}{2M}$. But the interacting ions lead to quantized elastic vibrations (phonons) with $\hbar\omega(\vec{k}) \sim C\hbar k$ – sound modes).

Wigner Crystal

Although we argued that e-e interactions are screened and so less important than one might expect, Wigner argued that the free-electron-like filled Fermi sphere ground state could become unstable to an insulating lattice of localized electrons, when the density of the electron gas gets sufficiently small. The formation of this Wigner electron crystal was proposed to be due to a competition between electrostatic potential energy and electron kinetic energy.

Wigner's arguement applies to a homogeneous electron gas with a fixed uniform neutralizing background of positive charge (ie instead of point positive ions). A simple argument is as follows.

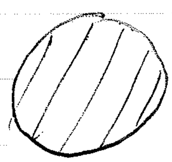
Consider the electrons localized to the points of a periodic lattice of sites. ~~Each electron occupies a volume~~ The volume per electron is $v = \frac{V}{N}$. We can imagine dividing the space up into spheres of radius r_s $\left(\frac{4}{3}\pi r_s^3 = v\right)$ with uniform positive charge filling the sphere and the electron at the center of the sphere. Of course such spheres may slightly overlap, and leave some voids in the regions where ~~they meet~~ neighboring spheres meet, but we ignore such complications for the sake of simplicity. Since each sphere is neutral, Gauss law gives that the $\vec{E}$ field out side each sphere will vanish, hence these spheres have little or no interaction between them. The electrostatic energy per electron is then just the electrostatic energy of the electron and ~~the~~ its uniform sphere of positive charge. On dimensional grounds we can estimate this energy as $-e^2/r_s$. Or we can do a calculation as follows:

Total electrostatic energy has two pieces

$$U = U_{ep} + U_{pp}$$

where U_{ep} is interaction of electron with positive charge ad U_{pp} is interaction of positive charge with itself.

We can get both by computing the electrostatic potential $V(r)$ due to the uniform sphere of positive charge.



charge density $\rho = \dfrac{e}{\frac{4}{3}\pi r_s^3}$

From ~~Gauss law~~ symmetry, $\vec{E}$ is radially symmetric ad in radial direction. Gauss law then gives for surface of radius r

$$\oint \vec{E}\cdot d\vec{a} = 4\pi r^2 E(r) = 4\pi \overbrace{\rho \tfrac{4}{3}\pi r^3}^{Q_{enclosed}} \qquad r < r_s$$

$$E(r) = \begin{cases} \frac{4}{3}\pi \rho r & r < r_s \\ \frac{e}{r^2} & r > r_s \end{cases}$$

substitute for ρ

$$E(r) = \begin{cases} \dfrac{\frac{4}{3}\pi e r}{\frac{4}{3}\pi r_s^3} = \dfrac{er}{r_s^3} & r < r_s \\ \dfrac{e}{r^2} & r > r_s \end{cases}$$

$$-\frac{dV}{dr} = E \Rightarrow \quad V(r) = \begin{cases} -\dfrac{er^2}{2r_s^3} + \text{const} & r < r_s \\ \dfrac{e}{r} & r > r_s \end{cases}$$

V continuous at $r = r_s$ $\Rightarrow$ $\text{const} - \dfrac{e}{2r_s} = \dfrac{e}{r_s}$

$$\text{const} = \frac{3}{2}\frac{e}{r_s}$$

$$V(r) = \begin{cases} \dfrac{e}{2r_s}\left\{3 - \dfrac{r^2}{r_s^2}\right\} & r < r_s \\ \dfrac{e}{r} & r > r_s \end{cases}$$

self energy of positive charge is

$$U_{pp} = \frac{1}{2}\int d^3r\, \rho V = \frac{4\pi}{2}\rho\int_0^{r_s} dr\, r^2 V(r)$$

$$= \frac{4\pi}{2}\frac{e}{\frac{4}{3}\pi r_s^3}\int_0^{r_s} dr\, \frac{e}{2r_s}\left\{3r^2 - \frac{r^4}{r_s^2}\right\}$$

$$= \frac{3}{4}\frac{e^2}{r_s^4}\left(r_s^3 - \frac{r_s^5}{5r_s^2}\right) = \frac{3}{4}\frac{e^2}{r_s^4} r_s^3 \frac{4}{5}$$

$$U_{pp} = \frac{3}{5}\frac{e^2}{r_s}$$

energy of electron - positive charge interaction is

$$U_{ep} = -eV(0) = \frac{-e^2 \, 3}{2r_s}$$

$$U = U_{ep} + U_{pp} = -\frac{e^2}{r_s}\left(\frac{3}{2} - \frac{3}{5}\right) = -\frac{e^2}{r_s}\left(\frac{15-6}{10}\right)$$

$$U = -\frac{9}{10}\frac{e^2}{r_s}$$

total electrostatic energy per electron of Wigner electron lattice.

We now have to add on the ~~tot~~ kinetic energy of the electron confined to the sphere of radius r_s.

A naive estimate of kinetic energy is as follows: For an electron in a sphere of radius r_s, ~~its wavefunctio~~ the wavelength of the wavefunction is $\lambda \sim r_s$

$\Rightarrow k = \frac{2\pi}{r_s}$ $\Rightarrow$ kinetic energy is $\frac{\hbar^2 k^2}{2m} \sim \frac{4\pi^2 \hbar^2}{2m r_s^2}$

Total energy per electron of Wigner lattice is

$$\mathcal{E}_W = -\frac{9}{10}\frac{e^2}{r_s} + 4\pi^2 \frac{\hbar^2}{2m r_s^2}$$

Compare this to the energy per electron of the filled Fermi sphere

$$\mathcal{E}_F = \frac{3}{5}\varepsilon_F$$

To compare these two energies

$$E_W = -\frac{9}{10}\frac{e^2}{a_0}\left(\frac{a_0}{r_s}\right) + \frac{4\pi^2}{2}\frac{\hbar^2}{me^2}\frac{e^2}{r_s^2}$$

use $a_0 = \frac{\hbar^2}{me^2}$

$$E_W = -\frac{9}{10}\frac{e^2}{a_0}\left(\frac{a_0}{r_s}\right) + 2\pi^2\frac{e^2}{a_0}\left(\frac{a_0}{r_s}\right)^2$$

$$= +\frac{e^2}{a_0}\left[-\frac{9}{10}\left(\frac{a_0}{r_s}\right) + 2\pi^2\left(\frac{a_0}{r_s}\right)^2\right]$$

whereas

from lecture 4

$$E_F = \frac{3}{5}\varepsilon_F = \frac{3}{5}\frac{e^2}{2a_0}(k_F a_0)^2 = \frac{3}{10}\frac{e^2}{a_0}(1.92)^2\left(\frac{a_0}{r_s}\right)^2$$

So the energy difference is

$$E_W - E_F = -\frac{e^2}{a_0}\left\{\frac{9}{10}\left(\frac{a_0}{r_s}\right) - 2\pi^2\left(\frac{a_0}{r_s}\right)^2 + \frac{6}{5}\left(\frac{a_0}{r_s}\right)^2\right\}$$

$$\simeq -\frac{e^2}{a_0}\left\{\frac{9}{10} - 18\left(\frac{a_0}{r_s}\right)\right\}\frac{a_0}{r_s}$$

So the Wigner lattice will have lower energy then the filled Fermi sphere (and hence will be the better ground state) when

$$E_W - E_F < 0 \Rightarrow \frac{9}{10} - 18\left(\frac{a_0}{r_s}\right) > 0$$

$$\Rightarrow \boxed{r_s > 20\,a_0}$$

So for sufficiently dilute electron gas, the Wigner lattice should become the ground state because the negative electrostatic energy outweighs the increase in kinetic energy.

The above was a rough ~~class~~ calculation. Clearly our estimate for both potential and kinetic energy terms for the Wigner lattice were rough estimates.

A more advanced calculation, using density functional method [Ceperley + Alder, PRL 45, 566 ~~(198)~~ (1980)] gives the critical value of r_s as

$$r_s \approx 100\, a_0$$