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 single argument is as follows.

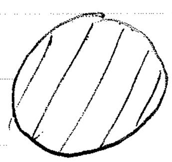
Consider the electrons localized to the points of a periodic lattice of sites. ~~Each electron occupies a volume~~ The volume per electron is $v = \frac{V}{N}$. We can imagine dividing the space up into spheres of radius r_s ($\frac{4}{3}\pi r_s^3 = v$) with uniform positive charge filling the spere 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 outside 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 and 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 and in radial direction. Gauss law then gives for surface of radius r

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

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

substitute for ρ

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

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

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

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

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

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, 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

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

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

$$E_F = \frac{3}{5}\varepsilon_F$$

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 than 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

$$r_s \approx 100\, a_0$$

Cooper pairing

An arbitrary weak but attractive interaction between two electrons excited above the filled Fermi surface leads to a bound state of the electrons with energy $E < 2\varepsilon_F$. This then leads to an instability of the filled Fermi sphere to such ~~pa~~ bound pair formation, that completely changes the nature of the ground state of the N-electron system and leads to the phenomenon of superconductivity (BCS - Bardeen-Cooper-Schrieffer theory of superconductivity). The presence of the filled Fermi sphere is crucial to the effect - compare to two isolated particles in 3D where a bound state will not form unless the interaction exceeds a certain strength.

Consider a pair of electrons excited above the Fermi surface ε_F. Assume that the ground state of this pair will have zero net momentum and zero net spin (singlet spin state). (Since the interaction is attractive $\Rightarrow$ ~~most fav~~ electrons prefer to be near each other $\Rightarrow$ most favorable wavefunction is spatially symmetric, so it must be antisymmetric in spin).

Let $\vec{r}_1$ and $\vec{r}_2$ be the positions of the two electrons. Assume that the two-particle wave function has the form:

$$\psi(r_1, r_2) = \frac{1}{V} \sum_k g_k e^{i\vec{k}\cdot\vec{r}_1} e^{-i\vec{k}\cdot\vec{r}_2} \qquad (V \text{ is volume})$$

ie $\vec{k}_1 = -\vec{k}_2$ so that ~~total~~ momentum of the pair is zero.

since we have a spin singlet (i.e. antisymmetric opposite spins), the real-space part of the wavefunction should be symmetric in exchange of r1 and r2. Hence we need g(k) = g(-k). We will see our solution will be consistent with this

Since the electrons are above a filled Fermi sphere we must have $g_k = 0$ for all $|\vec{k}| < k_F$ since these states are already occupied.

If $U(\vec{r}_1 - \vec{r}_2)$ is the interaction between the two electrons, then the Schrodinger equation is

$$-\frac{\hbar^2}{2m}\left[\nabla_1^2 + \nabla_2^2\right]\psi + U(\vec{r}_1 - \vec{r}_2)\psi = E\psi$$

Use Fourier transform $U(\vec{r}_1 - \vec{r}_2) = \frac{1}{V}\sum_q U_q e^{i\vec{q}\cdot(\vec{r}_1 - \vec{r}_2)}$

Plug into Schrodinger equation to get:

$$\frac{1}{V}\sum_k \frac{\hbar^2 k^2}{2m}\left[k^2 + k^2\right] g_k e^{i\vec{k}\cdot(\vec{r}_1 - \vec{r}_2)} + \frac{1}{V^2}\sum_{k' q} U_q e^{i\vec{q}\cdot(\vec{r}_1 - \vec{r}_2)} g_{k'} e^{i\vec{k}'\cdot(\vec{r}_1 - \vec{r}_2)}$$

$$= E \frac{1}{V}\sum_k g_k e^{i\vec{k}\cdot(\vec{r}_1 - \vec{r}_2)}$$

$$\Rightarrow \sum_k \left\{ \frac{\hbar^2 k^2}{m} g_k + \frac{1}{V}\sum_{k'} U_{k-k'} g_{k'} - E g_k \right\} e^{i\vec{k}\cdot(\vec{r}_1 - \vec{r}_2)} = 0$$

where we made substitution $\vec{q} = \vec{k} - \vec{k}'$ in the potential term

$$\Rightarrow \frac{\hbar^2 k^2}{m} g_k + \frac{1}{V}\sum_{k'} U_{k-k'}\, g_{k'} = E g_k$$
$$g_k = 0 \quad \text{for } |\vec{k}| < k_F$$
Bethe - Goldstone equation

using $\varepsilon_k = \frac{\hbar^2 k^2}{2m}$ we have

$$(E - 2\varepsilon_k) g_k = \frac{1}{V}\sum_{k'} U_{k-k'}\, g_{k'}$$

This is very difficult to solve for a general $U_{k-k'}$. To simplify, we make a crude approximation:

$$U_{k-k'} = \begin{cases} -U_0 & \text{if } \varepsilon_k, \varepsilon_{k'} \text{ within } \overbrace{\hbar\omega_D}^{\text{max phonon energy}} \text{ of } \varepsilon_F \\ 0 & \text{otherwise} \end{cases}$$

$$\Rightarrow g_k = \frac{-U_0 \left(\frac{1}{V}\sum'_{k'} g_{k'}\right)}{E - 2\varepsilon_k}$$

where Σ' means a sum over $\vec{k}'$ such that $|\vec{k}'| > k_F$ and $\frac{\hbar^2 k'^2}{2m} < \varepsilon_F + \hbar\omega_D$

Now sum both sides over $\vec{k}$

$$\left(\sum_k{}' g_k\right) = -U_0 \left(\frac{1}{V}\sum_{k'}{}' g_{k'}\right)\left(\sum_k{}' \frac{1}{E - 2\varepsilon_k}\right)$$

cancell $\Sigma' g_k$ from both sides to get

$$1 = -\mathcal{U}_0 \frac{1}{V} \sum_k{}' \frac{1}{E - 2\varepsilon_k}$$

$$\Rightarrow \quad 1 = -\mathcal{U}_0 \int_{\varepsilon_F}^{\varepsilon_F + \hbar\omega_D} d\varepsilon \, \frac{g(\varepsilon)}{E - 2\varepsilon}$$

$g(\varepsilon)$ is density of states.

$$\simeq -\mathcal{U}_0 \, g(\varepsilon_F) \int_{\varepsilon_F}^{\varepsilon_F + \hbar\omega_D} d\varepsilon \, \frac{1}{E - 2\varepsilon}$$

where we assumed $g(\varepsilon)$ varied slowly from ε_F to $\varepsilon_F + \hbar\omega_D$ (true since $\hbar\omega_D \ll \varepsilon_F$)

$$\Rightarrow \quad 1 = \frac{\mathcal{U}_0 g(\varepsilon_F)}{2} \ln\left(\frac{2\varepsilon_F - E + 2\hbar\omega_D}{2\varepsilon_F - E} \right)$$

solve above for the energy E

$$E = 2\varepsilon_F - \frac{2\hbar\omega_D}{e^{2/g(\varepsilon_F)\mathcal{U}_0} - 1}$$

For a weak potential, $\mathcal{U}_0 g(\varepsilon_F) \ll 1$, we have

$$E - 2\varepsilon_F = -2\hbar\omega_D \, e^{-2/g(\varepsilon_F)\mathcal{U}_0}$$

Since the pair of electrons, in the absence of the attractive potential $\mathcal{U}$, would have a minimum energy of $2\varepsilon_F$, the binding energy of the pair is

$$E' = 2\varepsilon_F - E = 2\hbar\omega_D \, e^{-2/g(\varepsilon_F)\mathcal{U}_0} > 0$$

$\Rightarrow$ bound state E has a lower energy than $2\varepsilon_F$

Note that the binding energy $\sim e^{-2/g(\varepsilon_F)U_0}$ is a non-analytic function of U_0, ie it cannot be expanded in powers of U_0. This means that we could never have gotten this result by using perturbation theory!

Conclusion: pairs of electrons at the Fermi surface ε_F can lower their energy by binding together into such a "Cooper pair". $\Rightarrow$ The filled Fermi sphere ~~can no longer~~ is unstable to the formation of Cooper pairs and so can no longer be the true ground state. The new ground state was obtained by B-C-S starting from this idea of Cooper pairs, and became the basis for understanding superconductivity. ✓

Back to the Cooper pair wavefunction:

$$g_k \sim \frac{U_0 \times \text{constant}}{2\varepsilon_k - E} \qquad \text{depends on } \vec{k} \text{ only via } \varepsilon_k$$

$\Rightarrow$ Solution is spherically symmetric $\Rightarrow$ Cooper pairs bind in an s-wave state.

The maximum g_k occurs for the smallest ε_k, ie at $|\vec{k}| = k_F$. Using $E = 2\varepsilon_F - E'$ we get

$$g_k \sim \frac{U_0}{2(\varepsilon_k - \varepsilon_F) + E'}$$

the distribution g_k as function of k has a width given by

$$\varepsilon_k - \varepsilon_F \simeq E' \ll \hbar\omega_D$$

Since only states within E' of ε_F are important in making the bound state, and $E' \ll \hbar\omega_D$, this suggests that the detailed structure of $U_{k-k'}$ is not so crucial and so our approximation might ~~not~~ be so terrible.

The size of a Cooper pair ~~is greater than~~ can be estimated as follows:

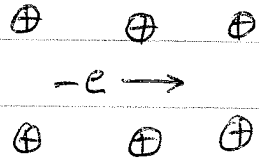
$$\xi_0 \sim \Delta R \sim \frac{1}{\Delta k} = \frac{1}{\frac{dk}{dE}\Delta E} = \frac{dE}{dk}\frac{1}{\Delta E} = \frac{\hbar v_F}{E'}$$

where we used that width in k-space was determined by $\varepsilon_k - \varepsilon_F \simeq E'$.

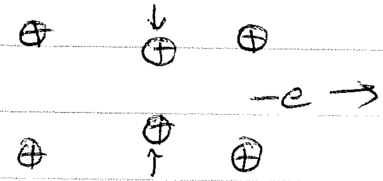
$$\xi_0 \sim \frac{\hbar v_F}{E'} \gg r_s \qquad \left(\tfrac{4}{3}\pi r_s^3 = \frac{1}{n}\right)$$

so the spatial extent of a Cooper pair is very much larger than the spacing between electrons

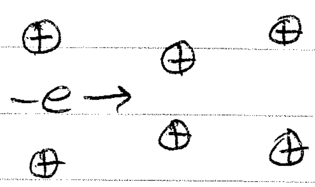
What is the origin of the attractive e-e interaction that leads to Cooper pairing?
It is a time-delayed ionic screening effect!



electron passes by



ions get attracted to electron and deform. Net (+) charge builds up where −e passed by, but now the −e electron has moved on!



the excess (+) charge where the ions have deformed then attracts a new electron to the place where the first electron had been. This leads to an effective (but time delayed) attrative correlation between the electrons.

Crucial to this picture is that the ions move much more slowly than the electrons, so the ion deformation that attracts the 2nd electron remains after the 1st electron has past. That is how the two (−) electrons can still attract!