Phys 726 - Lecture 6

Recap:

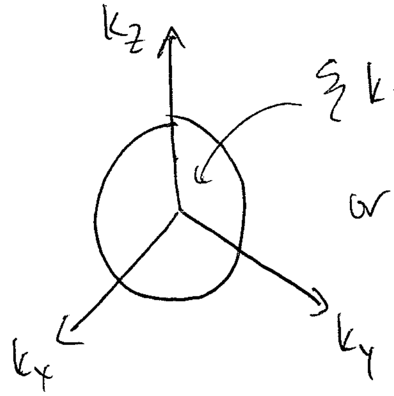
* We've been working through the formalism of the nonrelativistic quantum mechanics of

<u>many-particle</u> systems subject to <u>mutual interactions</u>

In the absence of interactions, the many-particle ground state is entirely determined by the particles' exchange statistics.

e.g. independent electrons settle into a Fermi Sea

$$|F\rangle = \left(\prod_{k<k_F} c^{\dagger}_{k\uparrow} c^{\dagger}_{k\downarrow} \right) |vac\rangle$$



$\{ k < k_F \}$

or $\left\{ \varepsilon_k = \dfrac{\hbar^2 k^2}{2m} < \varepsilon_F = \dfrac{\hbar^2 k_F^2}{2m} \right\}$

What these do depends on whether the interactions can be considered as weak or strong.

Possibility of destabilizing the Fermi Sea.

* We considered a tuneable Hamiltonian

$$\hat{H}(\lambda) = \hat{H}^{(1)} + \lambda \hat{H}^{(2)}$$

non-interacting one-body terms

adiabatic turn-on of two-body interaction terms

→ For fermions, $\hat{H}^{(1)}$ has a Fermi Sea ground state $|\Psi_{\lambda=0}\rangle = |F\rangle$

→ Imagine increasing λ from 0 to 1 arbitrarily slowly so that the ground state $|\Psi_\lambda\rangle$ evolves away from $|F\rangle$

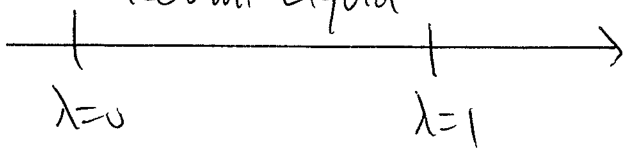
→ key question: Is there a critical value $0 < \lambda_c < 1$ above which $\langle F | \Psi_\lambda \rangle = 0$?

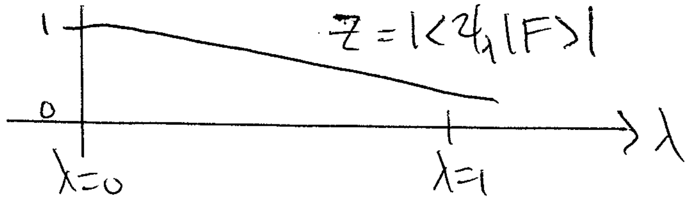
In other words, when we incorporate the interaction effects do we eventually achieve a state whose <u>character is fundamentally different</u> from the Fermi Sea

(different in what way? Can that be made precise?)

Weak interactions

Fermi Liquid





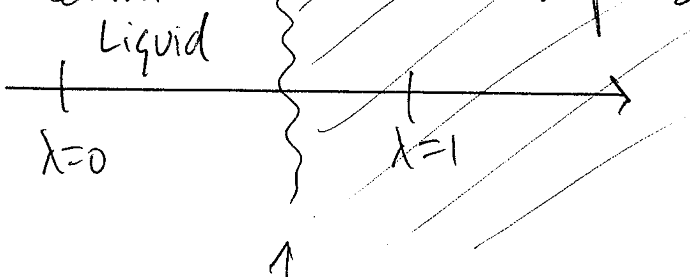
$|\psi_{\lambda=1}\rangle$, the true ground state of the interacting system, is adiabatically connected to $|\psi_{\lambda=0}\rangle = |F\rangle$

$$\boxed{\text{Perturbation Theory is under good control}}$$

Strong interactions

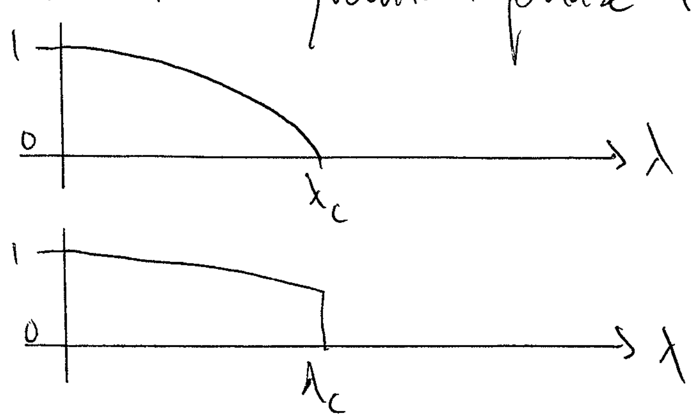
Fermi Liquid

Another phase: superconducting, magnetic, ...



quantum phase transition

$|\langle\psi_\lambda|F\rangle|$



$\boxed{\lambda_c \text{ defines a radius of convergence for any perturbative expansion around } \lambda=0}$

Plan for today:

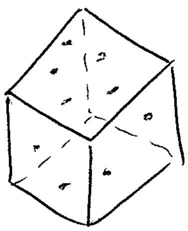
① Return to the example of the interacting electron gas in a uniform background of compensating charge (jellium model)

② Argue that perturbation theory (in r_s) must break down at low electronic density ($r_s \to \infty$) because of the appearance of the Wigner crystal (freezing of the Fermi Liquid into a "Fermi Solid")

③ Propose an alternative magnetic ground state at intermediate densities and justify its stability using a variational calculation

④ Use symmetry and symmetry-breaking as a framework for understanding the effects of strong interactions

Degenerate Electron Gas



N electrons confined to a volume V with uniform background charge of density $\rho(\vec{r}) = +\frac{eN}{V} = \text{const.}$

* two natural length scales
  - $\rightarrow$ interparticle spacing r_0, defined by $V = \frac{4}{3}\pi r_0^3 N$
  - $\rightarrow$ Bohr radius $a_0 = \frac{\hbar^2}{me^2}$

* density regime determined by the dimensionless parameter $r_s = r_0/a_0$

* rescaled Hamiltonian

$$\hat{H} = \sum_{k,\alpha} \frac{\hbar^2 k^2}{2m} c^\dagger_{k\alpha} c_{k\alpha} + \frac{e^2}{2V} \sum_{\substack{kk' \\ q\neq 0}} \sum_{\alpha\beta} \frac{4\pi}{q^2} c^\dagger_{k+q,\alpha} c^\dagger_{k'\beta} c_{k'+q\beta} c_{k\alpha}$$

$$= \frac{e^2}{a_0} \cdot \frac{1}{2r_s^2} \hat{A} + \frac{e^2}{a_0} \frac{2\pi}{\bar{V} r_s} \hat{B} = \frac{e^2}{2a_0} \frac{1}{r_s^2} \left(\hat{A} + \frac{4\pi}{\bar{V}} r_s \hat{B} \right)$$

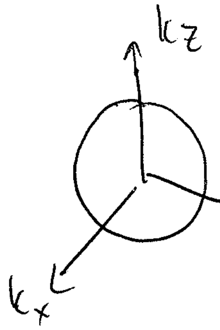
* Ground state energy expansion

$$E = \frac{Ne^2}{2a_0}\cdot\frac{1}{r_s^2}\left(\underset{\langle F|\hat{A}|F\rangle}{2.21} - \underset{\frac{4\pi}{V}\langle F|\hat{B}|F\rangle}{0.916\, r_s} + \underbrace{c_2 r_s^2 + \tilde{c}_2 r_2^2 \log r_s + \cdots}_{\text{"correlation energy contributions"}}\right)$$

= perturbative contributions at second order and higher

Unperturbed ground state energy

$$E_0 = \langle F|\hat{H}_{el}^{(1)}|F\rangle = N\cdot\frac{\int_0^{k_F} k^2 dk\, \frac{\hbar^2 k^2}{2m}}{\int_0^{k_F} k^2 dk} = \frac{3}{5}\frac{\hbar^2 k_F^2}{2m}\cdot N$$



integrating fermi sea in spherical shells

$$= N\cdot\frac{e^2}{2a_0}\cdot\frac{2.21}{r_s^2}$$

* First-order energy shift

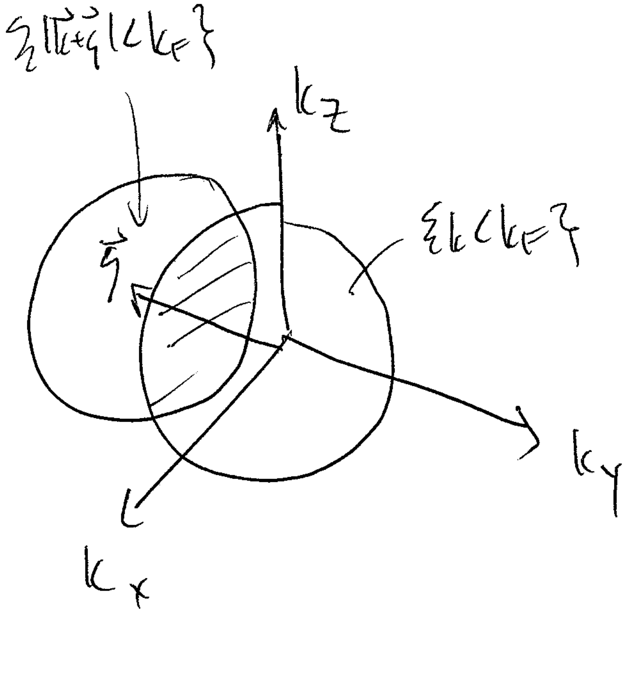
$$\Delta E = \langle F | \hat{H}_{el}^{(2)} | F \rangle$$

direct $\sim \delta_{q,0}$

$$= \frac{e^2}{2V} \sum_{\alpha\beta} \sum_{\substack{kk' \\ q \neq 0}} \frac{4\pi}{q^2} \langle F | c^\dagger_{k+q,\alpha} c^\dagger_{k'\beta} c_{k'+q\beta} c_{k,\alpha} | F \rangle$$

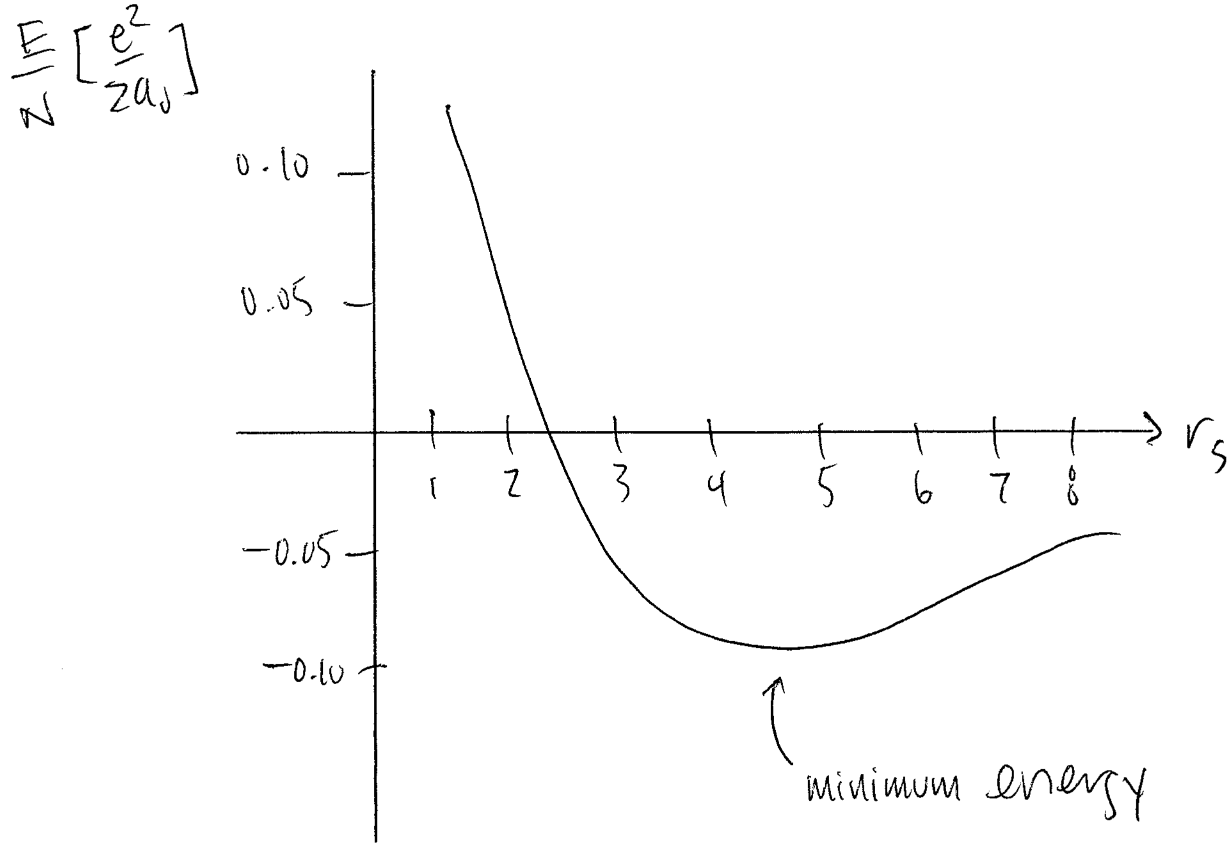
exchange

$$= -\frac{e^2}{2V} \sum_{\alpha} \sum_{k, \vec{q} \neq 0} \frac{4\pi}{q^2} \theta(k_F - |\vec{k}+\vec{q}|)\, \theta(k_F - k)$$



$$= -\frac{e^2}{2a_0} \cdot N \cdot \frac{0.916}{r_s}$$

minus sign because of fermion exchange



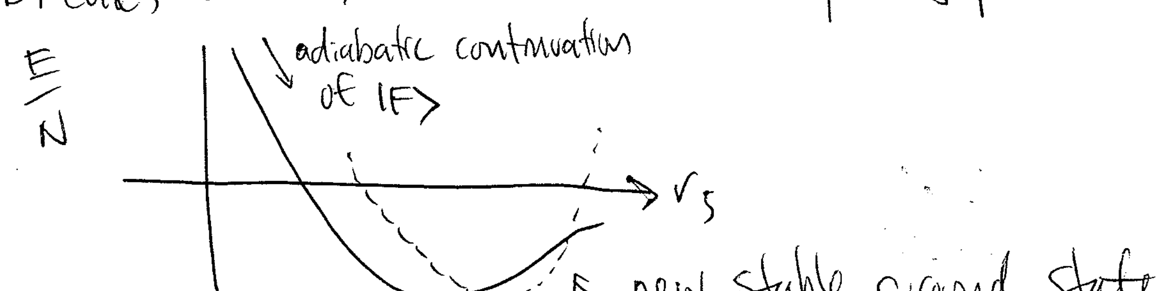
$$\frac{E}{N} = -0.095\,\frac{e^2}{2a_0} = -1.29\,eV$$

at $r_s = 4.83$

⇒ cohesion in the overall charge-neutral system

⇒ justifies the existence of condensed phases of matter !

* How large can we go in r_s before this picture breaks down? Are there competing phases ?



* Energy expansion

$$E = \frac{Ne^2}{2a_0} \cdot \frac{1}{r_s^2} \left(2.21 - 0.916 + \cdots \right)$$

$$= E_0 + \Delta E + \text{additional corrections at higher order}$$

$$= \langle F | \hat{H}_{el}^{(1)} | F \rangle + \langle F | \hat{H}_{el}^{(2)} | F \rangle + \cdots$$

$$= \langle F | \hat{H}_{el} | F \rangle + \cdots$$

view instead as the variational energy $E[|F\rangle] = \langle F | \hat{H}_{el} | F \rangle$

* We want to argue that there is another state $|W\rangle$ such that

$$E[|W\rangle] < E[|F\rangle] \text{ at large } r_s$$

Wigner crystal

* Start from viewpoint of $r_s = \infty$ rather than $r_s = 0$

$$\hat{H} = \frac{e^2}{2a_0}\left(\frac{1}{r_s^2}\hat{A} + \frac{4\pi}{V}\frac{1}{r_s}\hat{B}\right)$$

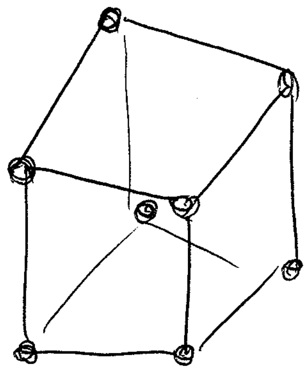
kinetic energy is negligible

low-electron-density limit is Coulomb dominated

→ In a gas, electrons move everywhere and can be arbitrarily close to one another

→ In a crystal arrangement the electrons are separated by $\sim r_0$ and gain potential energy $\sim \frac{e^2}{r_0}$

Most favorable arrangement is body-centered cubic (bcc)



unit cell with one electron at each cube vertex and one at the center

Electrostatic energy of the electron lattice

is $\frac{1}{2N} \sum_{\vec{R}\vec{R}'}' \frac{e^2}{|\vec{R}-\vec{R}'|} = \frac{1}{2} \sum_{\vec{R}\neq 0} \frac{e^2}{R}$ (a non-alternating version of the Madelung sum)

$$E_{Wigner} = \underbrace{\frac{1}{2} \sum_{\vec{R}\neq 0} \frac{e^2}{R}}_{\text{lattice}} - \underbrace{\frac{1}{2} \int \rho \frac{e^2}{r} d^3r}_{\text{positive background}}$$

$$= \frac{e^2}{2a_0} N \left[-\frac{1.79}{r_s} + \frac{2.66}{r_s^{3/2}} + \cdots \right]$$

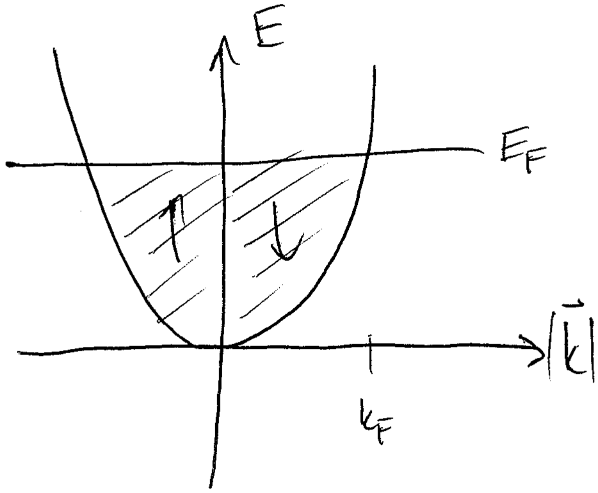
$E[|W\rangle] < E[|F\rangle]$ for $r_s \gtrsim 106$ (QMC)

Itinerant Ferromagnetism

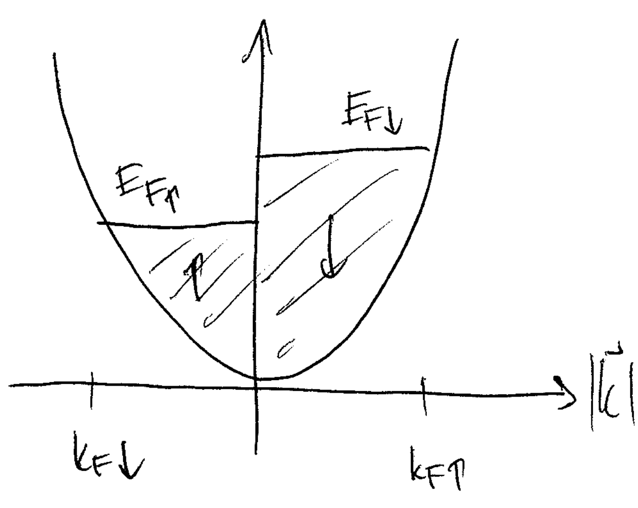
* So far, we've considered the spin degrees of freedom to be inert

→ $\sum_{\alpha=\uparrow,\downarrow}$ gives 2 identical contributions

due to equal spin-up and spin-down populations



→ but what about a spin-polarized system?



$$E_0 = \langle F' | \hat{H}^{(1)} | F' \rangle$$

with

$$|F'\rangle = \left(\prod_{k<k_{F\uparrow}} c^{\dagger}_{k\uparrow}\right)\left(\prod_{k<k_{F\downarrow}} c^{\dagger}_{k\downarrow}\right)|\text{vac}\rangle$$

$$N_\uparrow = \langle F' | \sum_k c_{k\uparrow}^\dagger c_{k\uparrow} | F' \rangle$$

$$= V \int \frac{d^3k}{(2\pi)^3} \theta(k_{F\uparrow} - k) = \frac{V}{8\pi^3} \int_0^{k_{F\uparrow}} 4\pi k^2 dk = \frac{V}{2\pi^2} \cdot \frac{1}{3} k_{F\uparrow}^3$$

or $$k_{F\uparrow} = \left(6\pi^2 \frac{N_\uparrow}{V}\right)^{1/3} \equiv \left(6\pi^2 n_\uparrow\right)^{1/3}$$

Similarly $$k_{F\downarrow} = \left(6\pi^2 \frac{N_\downarrow}{V}\right)^{1/3} \equiv \left(6\pi^2 n_\downarrow\right)^{1/3}$$

Then, the total kinetic energy is

$$E_0 = \langle F' | \sum_k \sum_\alpha c_{k\alpha}^\dagger c_{k\alpha} | F' \rangle$$

$$= \frac{V}{8\pi^3} \int_0^{k_{F\uparrow}} 4\pi k^2 dk \cdot \frac{\hbar^2 k^2}{2m} + \frac{V}{8\pi^3} \int_0^{k_{F\downarrow}} 4\pi k^2 dk \cdot \frac{\hbar^2 k^2}{2m}$$

$$= \frac{(6\pi^2)^{5/3}}{20\pi^2 m} \left[\left(\frac{N_\uparrow}{V}\right)^{5/3} + \left(\frac{N_\downarrow}{V}\right)^{5/3} \right]$$

population imbalance

Let $n = \frac{N}{V} = n_\uparrow + n_\downarrow$ and $\delta n = n_\uparrow - n_\downarrow$

So that $\frac{N_\uparrow}{V} = \frac{n + \delta n}{2}$ and $\frac{N_\downarrow}{V} = \frac{n - \delta n}{2}$

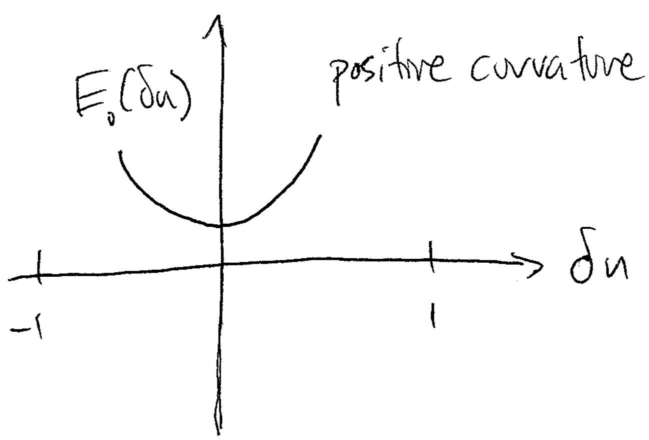
Note that

$$(n+\delta n)^{5/3} + (n-\delta n)^{5/3}$$

$$= n^{5/3}\left[\left(1+\frac{\delta n}{n}\right)^{5/3} + \left(1-\frac{\delta n}{n}\right)^{5/3}\right]$$

$$= n^{5/3}\left[2 + \frac{10}{9}\left(\frac{\delta n}{n}\right)^2 + O\left(\frac{\delta n}{n}\right)^4\right]$$

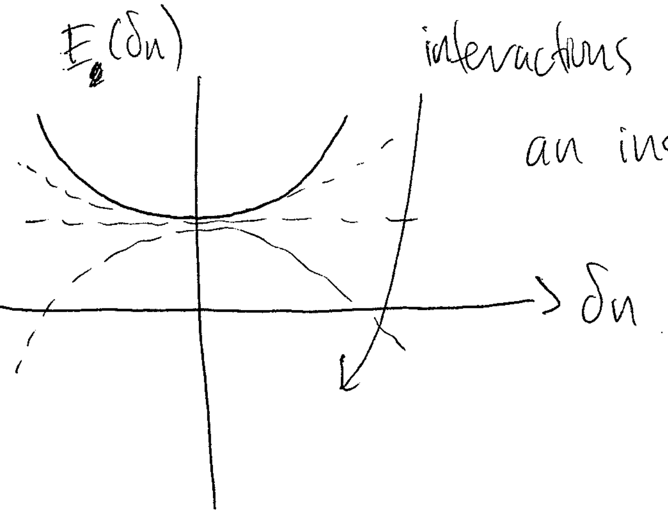
So $E_0(\delta n) = E_0(0) + (\text{positive constant}) \cdot \delta n^2$



positive curvature $\Rightarrow$ stability

state flows to $\delta n = 0$

The paramagnetic Fermi Sea does not polarize spontaneously at small r_s



interactions may generate an instability at larger r_s