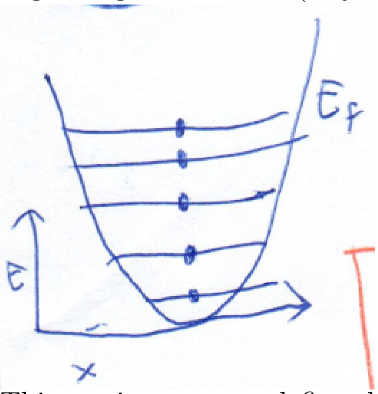
Week 10

PHY 635 Many-body Quantum Mechanics of Degenerate Gases
Instructor: Sebastian Wüster, IISER Bhopal, 2019

These notes are provided for the students of the class above only. There is no warranty for correctness, please contact me if you spot a mistake.

4.8 Trapped Atomic Fermi Gases

Now we explore the ultra-cold atomic Fermi gas further, within a harmonic trap, but initially neglecting interactions (as justified in section 4.7). We then find



left: Non-interacting ground state: All single particle states $|\varphi_n\rangle$ up to $E = E_F$ are filled with exactly one atom (or $(2S+1)$ atoms if we consider them to have spin S).

This motivates us to define the

Fermi-Sea State:

$$|FS\rangle_N = \prod_{n=0}^{N-1} \hat{a}_n^\dagger |0\rangle \tag{4.19}$$

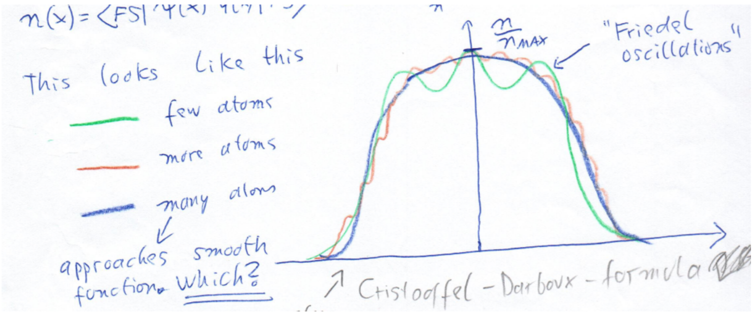
N = Atom-number and $E_n < E_F(N)$

Using the Fermi-field operator

$$\hat{\Psi}(x) = \sum_n \varphi_n(x)\hat{a}_n, \tag{4.20}$$

we obtain a total density

$$n(x) = \langle FS|\hat{\psi}^\dagger(x)\hat{\psi}(x)|FS\rangle \underset{\text{exercise}}{=} \sum_n |\varphi(x)|^2. \tag{4.21}$$



left: Results of (4.21) are plotted on the left for different numbers of atoms. The oscillations visible for smaller N are called Friedel Oscillations.

4.8.1 Thomas-Fermi-approximation

To find the density shape shown as the blue line (for many atoms) in the figures above, we can again use the Thomas-Fermi approximation, see section 3.3.4, however in a slightly different formulation.

Let us assume a large gas, so that we can use the local density approximation. This means we use the results derived in section 4.1, which were assuming a homogeneous system, by instead inserting a slowly varying density $N/V \to n(r)$.

From Eq. (4.6) and Eq. (4.8) we can then find relations between a local Fermi wavenumber/momentum and density and local Fermi-energy, as:

$$n(r) = \underbrace{\frac{k_F^3(r)}{6\pi^2}}_{\text{(ignoring spin)}}, \qquad \varepsilon_F(r) = \frac{\hbar^2 k_F(r)^2}{2m}. \tag{4.22}$$

The equillibrium density is such that adding one more atom has the same energy everywhere, thus:

$$\underbrace{\frac{\hbar^2 k_F^2(r)}{2m}}_{\substack{\text{added on} \\ \text{Fermi surface}}} + \underbrace{V(r)}_{\text{trap}} = \mu \tag{4.23}$$

Solving for $n(r)$ gives us the

Thomas-Fermi profile for Fermi gas

$$n(r) = \frac{1}{6\pi^2}\left(\frac{2m}{\hbar^2}[\mu - V(r)]\right)^{\frac{3}{2}} \quad \text{if} \quad \mu > V(r) \quad \text{else} \quad n(r) = 0 \tag{4.24}$$

- This gives the blue line in the previous figure.
- Note for BEC we have $[\mu - V(r)]^1$.

We can extend this local semiclassical/like WKB approach to include the momentum distribution and finite temperature effects with the resultant

Semiclassical distribution function for a Fermi gas:

$$f(\mathbf{r},\mathbf{p}) = \frac{1}{\exp[\beta(\frac{\mathbf{p}^2}{2m} + V(\mathbf{r}) - \mu)] + 1} \tag{4.25}$$

- From this we can obtain the total atom number

$$N = \frac{1}{(2\pi\hbar)^3}\int d^3\mathbf{r}d^3\mathbf{p}f(\mathbf{r},\mathbf{p}) \tag{4.26}$$

  or density/momentum density

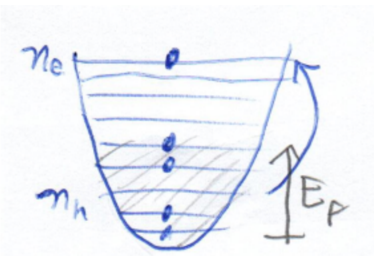
$$n(\mathbf{r}) = \frac{1}{(2\pi\hbar)^3}\int d^3\mathbf{p}f(\mathbf{r},\mathbf{p}) \tag{4.27}$$

$$\tilde{n}(\mathbf{p}) = \frac{1}{(2\pi\hbar)^3}\int d^3\mathbf{r}f(\mathbf{r},\mathbf{p}) \tag{4.28}$$

- The same view-point adopted here can give the Thomas-Fermi profile for bosons, derived with different methods for Eq. (3.46). In a (locally) homogeneous BEC there is no kinetic energy, but instead interaction energy $U_0 n(r)$, unlike the Fermionic case. Replacing in Eq. (4.23) the Fermi-(kinetic) energy $\frac{\hbar^2 k_F^2(r)}{2m}$ by $U_0 n(r)$, we then find Eq. (3.46).

4.8.2 Excitations of the ideal gas

The simplest excited state of $|FS\rangle$ is obtained, when we move any atom with $E < E_F$ to $E > E_F$.



left: Excitation of a degenerate Fermi gas, an atom has jumped from state n_h (h for hole) to n_e (e for excited).

In this we are actually doing two things: creating a hole at n_h (oscillator quantum number) and excited atom at n_e.

We can consider these both separately as excited states of a system with $N-1$ atoms (for the hole) or $N+1$ atoms (for the excited atom). Energy of hole: $E[\hat{a}_{n_h}|FS\rangle_N] - E[|FS\rangle_{N-1}] = E_F - E_{n_h} = E_F - \hbar\omega(n_h + \frac{1}{2})$

Similarly for excitation $\quad E[\hat{a}^\dagger_{n_e}|FS\rangle_N] - E[|FS\rangle_{N+1}] = E_{n_e} - E_F$

If we denote by n_F the oscillator state quantum number up to which all states are filled in the Fermi sea, we have

Energy of particle or hole excitation

$$E_n = \hbar\omega|n - n_F| \tag{4.29}$$

(homogeneous system would have $\varepsilon_k = \frac{\hbar^2|k^2-k_F^2|}{2m}$)

4.9 (Weak) Repulsive interactions in spin mixtures

- So far, we only considered non-interacting Fermi gases, which as per the discussion in section 4.7, is actually realistic for a cold single species gas.
- For two species (e.g. $\frac{N}{2}$ atoms in one spin state $|\uparrow\rangle$ and $\frac{N}{2}$ atoms in another $|\downarrow\rangle$) interactions become relevant since $|\uparrow\rangle$ atoms do have s-wave interactions with $|\downarrow\rangle$ atoms.
- Thus also evaporative cooling works again.
- Let us assume interactions are fully repulsive everywhere, that is $U(r) > 0 \quad \forall r$.

4.9.1 Landau Fermi Liquid

Let us consider "slow" turning on of interactions, so we start with perturbation theory. We use the

Hamiltonian for spin-mixture of a Fermi-gas

$$\hat{H} = \int d^3\mathbf{x}\Big\{\sum_{s=\uparrow,\downarrow} \hat{\psi}_s^\dagger(\mathbf{x})H_0\hat{\psi}_s(\mathbf{x}) + U_0\hat{\psi}_\uparrow^\dagger(\mathbf{x})\hat{\psi}_\downarrow^\dagger(\mathbf{x})\hat{\psi}_\downarrow(\mathbf{x})\hat{\psi}_\uparrow(\mathbf{x})\Big\}. \tag{4.30}$$

- The field operator now has a spin index

$$\hat{\psi}_s(\mathbf{x}) = \sum_n \hat{a}_{s,n}\,\varphi_n(\mathbf{x})\chi_s$$

($\chi_s =$ spinor i.e. $s = \ \uparrow \ \longrightarrow \begin{pmatrix}1\\0\end{pmatrix}$ and $s = \ \downarrow \ \longrightarrow \begin{pmatrix}0\\1\end{pmatrix}$)

($\hat{a}_{s,n}|0\rangle = |n,s\rangle$, $\quad n \to$ trap single particle state, $\qquad s = |\uparrow\rangle, |\downarrow\rangle$)

- We have,

$$\{\hat{\psi}_s(\mathbf{x}), \hat{\psi}_{s'}^\dagger(\mathbf{x}')\} = \delta_{ss'}\delta^{(3)}(\mathbf{x}-\mathbf{x}'). \tag{4.31}$$

- The Hamiltonian already includes the fact that only atoms in two different spin-states can interact, see section 4.7.

For simplicity, we only consider a homogeneous system, with the following expansion for the

Fermion field operator:

$$\hat{\psi}_s(\mathbf{x}) = \sum_{\mathbf{k}} \frac{\hat{a}_{s,\mathbf{k}}}{\sqrt{2\pi}^3} \underbrace{\varphi_{\mathbf{k}}(\mathbf{x})}_{planewaves} \chi_s, \quad \varphi_{\mathbf{k}}(\mathbf{x}) = \frac{1}{\sqrt{\mathcal{V}}} e^{i\mathbf{kx}}, \tag{4.32}$$

where $\mathcal{V}$ is a box-normalisation factor.

Using

$$(2\pi)^3 \delta^3(\mathbf{x}) = \int d^3\mathbf{x}\, e^{i\mathbf{kx}}$$

we obtain,

Momentum-space Hamiltonian for the spin-mixture

$$\hat{H} = \underbrace{\sum_k \frac{\hbar^2 k^2}{2m} (\hat{a}^\dagger_{\uparrow k} \hat{a}_{\uparrow k} + \hat{a}^\dagger_{\downarrow k} \hat{a}_{\downarrow k})}_{\hat{H}_0} + \underbrace{\frac{U_0}{\mathcal{V}} \sum_{\substack{k_1,k_2,k_3,k_4: \\ \mathbf{k}_1+\mathbf{k}_2=\mathbf{k}_3+\mathbf{k}_4}} \hat{a}^\dagger_{\uparrow k_3} \hat{a}^\dagger_{\downarrow k_4} \hat{a}_{\downarrow k_2} \hat{a}_{\uparrow k_1}}_{\hat{V}} \tag{4.33}$$

From this Hamiltonian, let us first find the energy of the unperturbed/ non-interacting Fermi-sea itself. The expectation value is

$$\begin{aligned} E^{(0)} =& \langle FS| \sum_k \frac{\hbar^2 k^2}{2m} (\hat{a}^\dagger_{\uparrow k} \hat{a}_{\uparrow k} + \hat{a}^\dagger_{\downarrow k} \hat{a}_{\downarrow k}) |FS\rangle \qquad (\hat{H}_0 \quad \text{only!}) \\ =& (4\pi) \int_0^{k_{F,\uparrow}} dk k^2 \underset{\substack{\downarrow \\ \text{density} \\ \text{of states}}}{D} \frac{\hbar^2 k^2}{2m} + (4\pi) \int_0^{k_{F,\downarrow}} dk k^2 D \frac{\hbar^2 k^2}{2m} \\ \underset{\substack{Eq.\ (4.6), Eq.\ (4.8) \\ D=\mathcal{V}/(2\pi)^3}}{=} & \frac{3}{5} (E_{F\uparrow} N_\uparrow + E_{F\downarrow} N_\downarrow) \end{aligned}$$

In the second equality, we used the fact that number operators give 0 for wave-numbers above the Fermi-level and 1 below. Then we also already did the angular integration in spherical 3D coordinates for $\mathbf{k}$. Since energies are apparently separately found for each spin species, we have also derived the

Total energy of an ideal Fermi gas

$$E_{Tot} = \frac{3}{5} E_F N \tag{4.34}$$

Now let us find the change of the energy due to some small interactions U_0 using Rayleigh-

Schödinger perturbation theory. The first order energy correction, as usual, is:

$$E^{(1)} = \langle FS|\hat{V}|FS\rangle \underset{\substack{k_1=k_3,\\ k_2=k_4}}{=} \frac{U_0}{V}\sum_{k_1,k_2}\langle \hat{a}^\dagger_{\uparrow k_1}\hat{a}_{\uparrow k_1}\rangle\langle \hat{a}^\dagger_{\downarrow k_2}\hat{a}_{\downarrow k_2}\rangle = \frac{U_0}{V}N_\uparrow N_\downarrow \tag{4.35}$$

Below the first equality, we indicate that for a non-vanishing matrix elements, indices in $\hat{V}$ have to be equal as shown. We show (4.35) here mainly as example for perturbation theory in a many-body context.

Let us also look in the first order correction to the quantum state $|\,FS\,\rangle$:

The formula you know from basic quantum mechanics perturbation theory is:

$$\underbrace{|n^{(1)}\rangle}_{\text{perturbed state}} = \sum_{k\neq n}\frac{\langle\, k^{(0)}\,|\hat{V}\overbrace{|\,n^{(0)}\,\rangle}^{\text{unpert. state}}}{E_n^{(0)}-E_k^{(0)}}\underbrace{|k^{(0)}\rangle}_{\text{basis}} \tag{4.36}$$

In our many-body context this translates to

$$|\,FS^{(1)}\,\rangle = \sum_{\mathbf{N}}{}' \frac{\langle\,\mathbf{N}\,|\hat{V}|\,FS^{(0)}\,\rangle}{E^{(0)}-E_{\mathbf{N}}}|\,\mathbf{N}\,\rangle \tag{4.37}$$

- The prime $'$ on the sum shall denote that the sum does not include the state $|\,FS\,\rangle$ itself.
- We use Fock-states $|\,\mathbf{N}\,\rangle$, see Eq. (2.2), for Fermions, taking into account occupations of different spin states also.
- We find

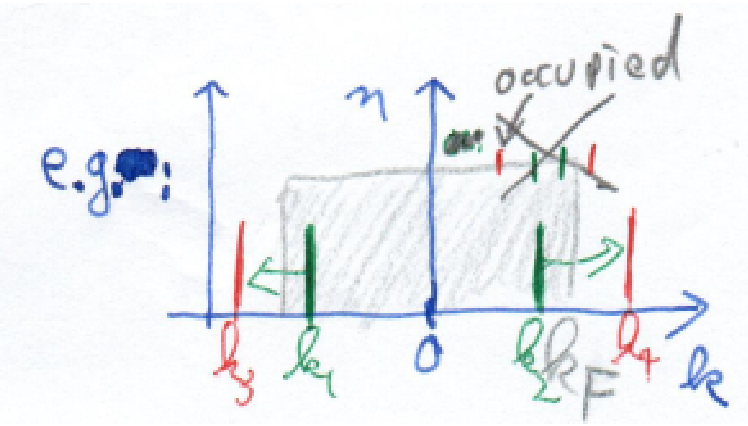
$$E_{\mathbf{N}} = \sum_k \frac{\hbar^2k^2}{2m}(N_{k\uparrow}+N_{k\downarrow})$$

- For $\hat{V}$, see Eq. (4.33).

Let's evaluate the required Matrix elements:

$$\langle\,\mathbf{N}\,|\hat{V}|\,FS^{(0)}\,\rangle = \frac{U_0}{V}\sum_{\substack{k_1,k_2,k_3,k_4:\\ \mathbf{k}_1+\mathbf{k}_2=\mathbf{k}_3+\mathbf{k}_4}} \underbrace{\langle\,\mathbf{N}\,|\hat{a}^\dagger_{\uparrow k_3}\hat{a}^\dagger_{\downarrow k_4}\underbrace{\hat{a}_{\downarrow k_2}\hat{a}_{\uparrow k_1}|\,FS^{(0)}\,\rangle}_{\text{we need}\quad |k_1|,|k_2|<k_F}}_{\substack{\text{we need}\quad k_1=k_3,k_2=k_4\\ \text{Or,}\quad |k_3|,|k_4|>k_F}} \tag{4.38}$$

Below the braces we indicate conditions for operators acting on states to gives something non-zero. One choice, $k_1 = k_3$, $k_2 = k_4$ is boring, because we end up coupling $|\,FS\,\rangle$ with itself. However for the second choice $|k_3|, |k_4| > k_F$ we mix $|\,FS\,\rangle$ with the "double particle-hole excitation" state sketched below:



left: Double particle-hole excitation: A state with the filled Fermi sea, but then two atoms at momenta k_1 and k_2 were removed, and lifted above the Fermi surface to k_3 and k_4.

Let us give this is definition:

Particle-hole state

$$|\ \underbrace{(k_3\uparrow)^e}_{\substack{\text{excitation with}\\ \text{wave-vector } \mathbf{k}_3}}\ (k_4\downarrow)^e\ \ (k_2\downarrow)^h\ \underbrace{(k_1\uparrow)^h}_{\substack{\text{hole with}\\ \text{wave-vector } \mathbf{k}_1}}\ \rangle \tag{4.39}$$

eg: spin$\uparrow$ spin$\downarrow$

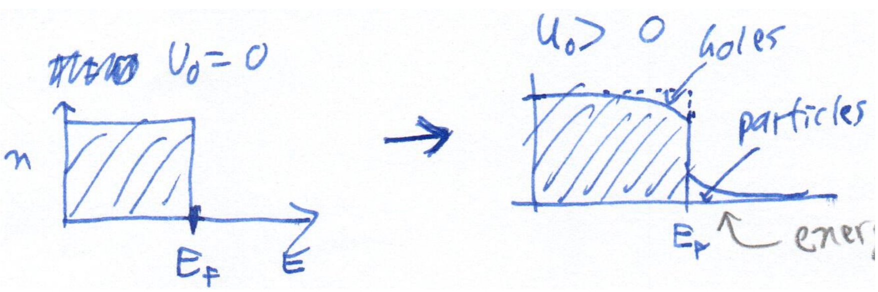
The perturbed Fermi-sea from Eq. (4.37) thus is

$$|\,FS^{(1)}\,\rangle = |\,FS^{(0)}\,\rangle + \frac{U_0}{V}\sum_{\mathbf{k}_1+\mathbf{k}_2=\mathbf{k}_3+\mathbf{k}_4}\frac{|\,(k_3\uparrow)^e(k_4\downarrow)^e(k_2\downarrow)^h(k_1\uparrow)^h\,\rangle}{E^{(0)}-[\sum_{l=1,\cdots,4}\frac{\hbar^2|k_l^2-k_F^2|}{2m}+E^{(0)}]} \tag{4.40}$$

It is said that the interactions dress the FS with particle+hole pairs: A

Fermi-liquid is a Fermi sea, which interactions dress with particle+hole pairs as in Eq. (4.40).

This leads to a softening/smearing out of the Fermi edge even at $T=0$:

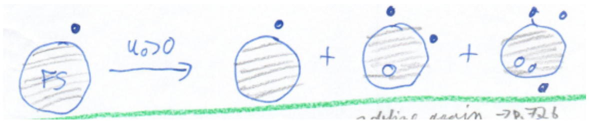


left: Fermion energy distribution without interactions (left), and with weak repulsive interactions (right), forming a Fermi-liquid. Particle and hole excitation becomes increasingly unlikely away from the Fermi surface, due to the energy denominator in (4.40).

Similarly to the ground-state, in the Fermi-liquid, also excited-states get dressed with other excited many-body states.

Fermi liquid theory can be understood as free fermions $|\, k, \underset{spin}{\sigma} \,\rangle$ evolving into fermionic quasi-particles with the same momentum and spin, due to interaction/dressing. These have a slightly modified effective mass m^*.

Quasi-particle cartoon:



- Most properties of Fermi-liquid system are (surprisingly) similar to the non-interacting cases.
- Applied to electrons in a metal, this describes most non-superconducting metals.
- Cold-atom experiments:
  See Nascimbine et al. Nature 463 1057 (2010).
  Horikoshi et al. Science 327 442 (2010).