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

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4 Degenerate Fermi Gases

4.1 Ideal Fermi Gases

Week (9)

In section 3.2 we explored what happens to N non-interacting <u>Bosons</u> as the temperature is decreased $T \downarrow 0$. Now we follow the same question for <u>Fermions</u>, thus using the Fermi-Dirac distribution [Eq. (3.11)]:

$$\bar{m}_b = \frac{1}{\exp[\beta(\varepsilon_b - \mu)] + 1}$$

- First difference: $\bar{m}_b > 0 \ \forall \varepsilon_b, \mu \to \text{no constraint on } \mu \text{ in contrast to Bose case.}$
- We can also much more easily take the limit

$$\lim_{T \to 0} \bar{m}_b = \begin{cases} +1 & \varepsilon_b < \mu \\ 0 & \varepsilon_b > \mu \end{cases}$$

• Let us plot Eq. (3.11) for various parameters



We see that for T = 0, all states with energy below μ are occupied, and above are not. This sharp transitions "softens" up, as we increase the temperature.

• We again find, that the Fermi-Dirac distribution approaches the classical Boltzmann distribution, once states are weakly occupied $(m_n \ll 1 \rightarrow \exp[\cdots] \gg 1)$ and energies much higher than μ .

It is clear in the plot above, that $E = \mu$ seems to be a special energy. To figure out what it means, lets look at non-interacting Fermions in a 3D box potential of cube-side-length L with spin s $(|\vec{s}| = \frac{1}{2})$.



left: Particle in a cubic box: We recall that wave-numbers in trigonometric eigenfunctions $\sin(k_l x)$ are quantized in each spatial dimension with condition

$$\begin{aligned} k_l &= \frac{n_l \pi}{L} \\ l &\in \{x, y, z\} \\ n_l &= 1, 2, \dots \infty \end{aligned}$$

Let us first consider the T = 0 case. As before in our discussion of Bosons, μ sets the total (mean) number of particles according to

$$N = \sum_{\text{all states } b} \bar{m}_b \tag{4.1}$$

$$\Rightarrow N \stackrel{\text{here}}{=} \sum_{n_x, n_y, n_z, s} \bar{m}_{n_x, n_y, n_z, s}$$
(4.2)

At zero temperature, we have simply

$$\bar{m}_{n_x,n_y,n_z,s} = \begin{cases} 1 & E_{\mathbf{n}} < \mu \\ 0 & E_{\mathbf{n}} \ge \mu \end{cases}$$

where $E_{\mathbf{n}} = \frac{\mathbf{n}^2 \pi^2 \hbar^2}{2mL^2}$ is the particle in the box energy. Since the latter is always positive, we see the first important difference to the Bose case, that we require $\mu > 0$ in order to have any particles. Then

$$\Rightarrow N = \sum_{n_x, n_y, n_z, s} \bar{m}_{n_x, n_y, n_z, s} \approx \frac{2}{8} \int d^3 \mathbf{n} \ \bar{m}_{\mathbf{n}}$$
(4.3)

$$= \frac{4\pi}{4} \int_0^{n_{\text{max}}} dn \ n^2 \text{ (use 3D spherical coordinates)}$$
(4.4)

$$=\frac{1}{3}\pi n_{\max}^3\tag{4.5}$$

where $n_{\max} = \sqrt{\frac{2mL^2\mu}{\pi^2\hbar^2}}$. At the first \approx we approximate the sum by an integration. We get a factor of 2 from summation over the two spin-states $m_s = +1/2, -1/2$, and we get a factor of 1/8 since the original sum runs only over positive n_x, n_y, n_z , while the integration runs over all 8 sign quadrants. In the second line, we built in that \bar{m} will be zero for $|\mathbf{n}| > n_{\max}$

Altogether we obtained N as a function of μ and can then solve for μ to find the

Fermi-energy (for non-interacting $s = \frac{1}{2}$ Fermions in a box) $\mu_0 = E_F = (3\pi^2)^{2/3} \frac{\hbar^2}{2m} \left(\frac{N}{V}\right)^{2/3}, \ V = L^3$ (4.6)

- Thus at T = 0 (or for $k_B T \ll E_F$), the Fermions occupy all energy states up to (approx up to) E_F . See blue line (brown line) in the earlier figure. This configuration, where μ is somewhat more important for the distribution than T, is called degenerate Fermi gas (DFG).
- In phase space, the surface where particles have exactly the Fermi energy E_F , is called <u>Fermi surface</u>.
- The transition to a DFG is less sharp than for a BEC, roughly we can say that the <u>degeneracy</u> temperature to DFG is

$$k_B T \approx E_F \tag{4.7}$$

• Had we used only a single spin-state, the pre-factor would be $(3\pi^2)^{2/3} \rightarrow (6\pi^2)^{2/3}$, we shall require this later. We also define the

Fermi-momentum or Fermi-wavenumber via

$$\frac{\hbar^2 k_F^2}{2m} = \frac{p_F^2}{2m} = E_F, \text{ i.e. momentum at Fermi surface}$$

$$k_F = [(3\pi^2)\rho]^{1/3}, \ \rho = \frac{N}{V} \text{ (density)}$$

$$(4.9)$$

Examples:

<u>Electrons in a conductor</u>: Iron (Fe) has a mass density of $\rho \sim 7.8 \text{ g/cm}^3$, which gives roughly an atom number density of $\rho_{\text{Fe}} \approx 8.3 \times 10^{28} \text{/m}^3$. There are two conduction electrons

per atom, hence $\rho_{e^-} = 16.6 \times 10^{28}/\text{m}^3$. Using Eq. (4.7) and Eq. (4.6) we can find that $T_F \approx 1.3 \times 10^5 \text{K}$ and $E_F \approx 2\text{-}10 \text{ eV}$. \Rightarrow Conduction electrons are DFG at all reasonable temperatures (where the metal still exists).

<u>Cold Fermionic atoms</u>: E.g. ⁶Li. In atom traps (as discussed for BEC) the density is very low $\rho \approx 10^{17}/\text{m}^3$. Using the equations above, we find $T_F \approx 80$ nK, so this is again the same range of temperatures as for BEC. We shall later re-calculate E_F in a harmonic trap, see Eq. (4.17), which would be more appropriate for this case.

• We see that how cold is cold enough for degeneracy of Fermions strongly depends on the system.

4.2 Degeneracy Pressure

One consequence of populating all states up to energies E_F is that these particles may move "fast" and hence contribute to significant pressure.



left: pressure = elastic collisions off wall

Basic thermodynamic P, V, E relation

$$P \cdot V = \frac{2}{3} N \langle \varepsilon_{\rm kin} \rangle, \ P \to \text{Pressure}$$

For the DFG of particles in box

$$\langle \varepsilon_{\rm kin} \rangle = \frac{2}{8} \frac{\int d^3 \mathbf{n} \ E(\mathbf{n})}{N}, \quad \left(E(\mathbf{n}) = \frac{\mathbf{n}^2 \pi^2 \hbar^2}{2mL^2} \right)$$
$$= \frac{4\pi}{4} \left(\frac{\pi^2 \hbar^2}{2mL^2} \right) \frac{\int_0^{n_{\rm max}} dn \ n^4}{N}$$
$$\stackrel{=}{\underset{(\rm exercise)}{=}} \frac{3}{5} E_F$$

We arrive at the

Fermi-pressure , also called degeneracy pressure:

$$P_F = \frac{2}{5} \left(\underbrace{\frac{N}{V}}_{\rho} \right) E_F \sim \rho^{5/3} \tag{4.10}$$

- This is valid for $T \leq T_F$ and unlike the classical case, there is <u>non-zero pressure</u> all the way to T = 0.
- You can think of this as Fermions resisting being sqeezed into "same state". (But note, there are <u>no</u> interactions.)

4.3 Applications in Astrophysics

4.4 White dwarf stars

pressure due to ideal gas heat/

- In our sun, inward gravity is balanced by outward pressure and radiation pressure due to fusion reaction $H+H \rightarrow He$ sustaining temperature T.
- When fuel runs out, heavy stars shrink and get hotter, then do fusion of He \rightarrow C,...,Fe.
- The latter won't work for solar-mass star, because they are too light, so we can ask what happens when they run out of H, thus only contain He, and can no longer provide fusion? \Rightarrow In some cases we get a <u>white-dwarf</u> where gravity is balanced by Fermi-pressure (4.10).

Stellar DFG: Assume a compressed star with mass $M = 10^{30}$ kg, central density $\rho_{\text{center}} = 10^{10}$ kg/m³, temperature $T = 10^7$ K. [c.f Sun $M_{\odot} = 2 \times 10^{30}$ kg, $\rho_{\text{center}} = 1.6 \times 10^5$ kg/m³, $T = 1.57 \times 10^7$ K]. We assume the old star contains now only ionized Helium.

$$\Rightarrow M \approx N_{\text{elec}} m_{\text{e}} + N_{\text{nucleons}} m_{\text{p}}$$
$$= N_{\text{elec}} (m_{\text{e}} + 2m_{\text{p}})$$
$$\approx 2N_{\text{elec}} m_{\text{p}}$$

Estimate number density of electrons roughly (turns out, pressure by He nuclei is negligible),

$$\rho_{\rm e} = \frac{N}{V} = \frac{M/2m_{\rm p}}{M/\rho_{\rm center}} = \frac{\rho_{\rm center}}{2m_{\rm p}} \approx 3 \times 10^{-9} {\rm electrons/fm}^3$$

Fermi temperature $T_F \stackrel{Eq. (4.7)}{=} 8.8 \times 10^9 \text{ K}$ \Rightarrow Despite being very hot, electrons at these high densities form DFG!

Stable equilibrium radius R of star (simplify star as a <u>uniform</u> sphere):

$$0 = dE = \frac{\partial}{\partial R} \left(\underbrace{-\frac{3}{5} \frac{M^2}{R}}_{E_{\text{grav}}} \right) dR \underbrace{-P_F(R)(4\pi R^2 dR)}_{\text{using } dE = -PdV \text{ from thermodynamics}}$$
(4.11)

We can solve this for the

White-dwarf radius:	$R_* = \mathcal{N} \frac{\hbar^2}{Gm_{\rm e} m_{\rm He}^{5/3} M^{1/3}}$	(4.12)
	$R_* = \mathcal{N} \frac{\hbar^2}{Gm_{\rm e}m_{\rm He}^{5/3}M^{1/3}}$	(4.12)

• Here $\mathcal{N} = 3(6\pi^2)^{1/3} \approx 11.69$ is a numerical pre-factor. Proof: Assignment 5. Test: Sirius B, $M = 1.05M_{\odot}, R = 5100 \text{ km}$ (Formula (4.12) gives 7030 km)

4.4.1 Relativistic DFG

For very dense (massive) white dwarfs, e^- near the Fermi surface become so fast that they have to be treated relativistically. We have to recalculate section 4.1 and section 4.2 using

$$E_{\rm kin} = mc^2 \left(\sqrt{1 + \left(\frac{p}{mc}\right)^2 - 1} \right). \tag{4.13}$$

After a technical calculation, we find the relativistic Fermi-pressure

$$P_F \sim \text{const.} \cdot \rho^{4/3}$$
 (4.14)

If we redo 4.11 with this, we find there is no stable R_* for a stellar mass above the

Chandrasekhar-limit:

$$M \approx 1.44 M_{\odot} \tag{4.15}$$

where M_{\odot} is the solar mass. This is the maximal mass for white dwarf stars.

4.4.2 Neutron stars

- For heavier stars, e⁻ degeneracy pressure cannot halt gravitational collapse once fusion runs out.
- Once matter reaches density of $\rho \sim 10^{17}$ kg/m³ (density of nuclei), electrons and protons form neutrons via inverse beta decay



• At equal density, P_F from neutrons is $\frac{m_e}{m_p}$ times that of electrons, and thus intrinsically much smaller, see Eq. (4.6)-(4.10). However, at some point the density becomes so high that also the degeneracy pressure P_F of <u>neutrons</u> becomes relevant, and may halt collapse.

Neutron star:

The result, when all matter is converted to neutrons and neutron degeneracy pressure has halted gravitational collapse. Their typical mass range is

$$1.4M_{\odot} < M < 3M_{\odot},$$

with a radius of

 $R \sim 20 \mathrm{km}.$

If neutron Fermi-pressure is overcome as before in section 4.4.1 (by neutrons becoming relativistic) → total gravitational collapse, <u>black-hole</u>.

4.5 Electron gas in metals

• Alkali metals or Copper, Silver, Gold: 1 valence e⁻ per atom. Picture:



- Ions bound by "immersion" in electron gas (metallic binding)
- Electron-electron Coulomb interactions are <u>screened</u> due to background ion sea and hence weak
- Electron-ion interactions: electrons aren't really "free", but see periodic potential $V(\mathbf{x}) = V(\mathbf{x} + \mathbf{d})$

Bloch theorem: Eigenstates for electrons in the periodic ion potential are of the form

$$\phi_{\mathbf{k},j}(\mathbf{x}) = u_j(\mathbf{x})e^{i\mathbf{k}\cdot\mathbf{x}} \tag{4.16}$$

where $u_j(\mathbf{x}) = u_j(\mathbf{x} + \mathbf{d})$, i.e the function *u* possesses the same periodicity properties as the ionic potential $V(\mathbf{x})$

Gives rise to <u>band-structure</u>⁴ (note, energies for negative k are the same E(-k) = E(k)):





4.6 Ultra-cold atomic Fermi-gas

- As in section 3.2, we now focus on a dilute gas of ultra-cold atoms in a harmonic trap, but here now <u>fermionic atoms</u>.
- Recall that compound objects of an even number of constituent Fermions are Bosons, while those of an odd number of constituent Fermions are Fermions. Since all items making up

⁴Top band E(k) curve should be flipped.

andatom are Fermions (electrons and nucleons, or more fundamentally, electrons and quarks), we need $N_{\text{elec}} + N_{\text{protons}} + N_{\text{neutrons}}$ to be odd for a fermionic atom. Since $N_{\text{elec}} = N_{\text{protons}}$ for neutral atoms, the sum of the two is always even. Thus fermionic atoms are all those with an <u>odd number of neutrons</u>.

- We assume spin-polarization for now, (e.g all \uparrow).
- We neglect interactions (but show shortly this is even realistic when all | ↑)).
 Expected picture:



- At t = 0, $\overline{m}_b = 1$ up to $\mu = E_F$.
- Harmonic trap $E_{n_x,n_y,n_z} = \hbar \omega (n_x + n_y + n_z)$

 $\Rightarrow N(\mu) = \sum_{n_x, n_y, n_z} 1 \text{ (with } (n_x + n_y + n_z) < \frac{\mu}{\hbar\omega}) = \text{ Volume of the green object above}$ $= (\mu/\hbar\omega)^3/6$

With same reasoning as before, we obtain the



- Using numbers as for the degeneracy temperature of Bose-atoms earlier [after Eq. (3.14)], we obtain $T_F \approx 187$ nK (N = 10000, $\omega = (2\pi)100$ Hz)
- Seems slightly "easier" to reach than BEC, but making a degenerate Fermi gas of cold atoms turned out harder. <u>Reasons:</u>
 - (i) Evaporative cooling (see PHY402 p.89) relies on <u>interactions</u> for remnant atoms to rethermalize.

- (ii) Fermi-blocking (section 2.2.4): atom has to scatter exactly into the right "empty" state. We see in the next section that spin-polarized ultracold Fermions barely interact.
- <u>Solution</u>: e.g sympathetic cooling: mix Bosons and Fermions, cool Bosons, Fermions <u>can</u> interact with Bosons, thus cool down together.

4.7 Ultra-cold Fermion interactions

Let us revisit quantum scattering theory as in section 3.3.1.



The wavefunction corresponding to this cartoon is

$$\psi_0(\mathbf{r}) = \exp(ikz) + \frac{f(\theta)}{r}\exp(ikr)$$

where $\mathbf{r} = \mathbf{r}_B - \mathbf{r}_A$ is the relative coordinate between the two collision partners, and $r, \theta, (\varphi)$ the corresponding 3D spherical coordinates.

For <u>Fermions</u>, to fulfill the anti-symmetrisation requirement, we need $\psi(\mathbf{r}) \stackrel{!}{=} -\psi(-\mathbf{r})$. We could try the usual trick:

$$\psi(\mathbf{r}) = \frac{1}{\sqrt{2}} (\psi_0(\mathbf{r}) - \psi_0(-\mathbf{r})).$$
(4.18)

Note

$$\psi_0(-\mathbf{r}) = \exp(-ikz) + \frac{f(\theta + \pi)}{r} \exp(ikr).$$

But for S-wave scattering (see pg. 42), $f(\theta) = \text{const.}$ (indep. of θ), so construction doesn't work, because the scattering part of the wavefunction vanishes in (4.18). We would need $f(\theta) = -f(\theta+\pi)$, which would be true only for <u>P-wave scattering</u> (l = 1 relative angular momentum).

But our arguments to neglect \overline{P} -wave scattering in the ultra-cold regime in section 3.3.1. hold also for Fermions.

No s-wave scattering or identical Fermions \Rightarrow <u>Ultra-cold</u>, <u>spin-polarized</u> Fermions are to a very good approximation effectively non-interacting</u>.

- It implies that results such as Eq. (4.17) are actually useful.
- Importantly, the basic interatomic interaction potential as sketched in section 3.3.1 [Eq. (3.19)] would not be much different between Bosonic or Fermionic isotopes of the same atom. The statement above only arises <u>effectively</u> in ultra-cold scattering, since the Fermion symmetry of the many-body wave-function makes it less likely at cold temperatures for the two Fermions to be ever close to each other.
- The situation changes if we have 2 spin-states \uparrow , \downarrow , which can take care of symmetrization in (4.18) \Rightarrow then S-wave interactions are possible.