

# PHY635, II-Semester 2022/23, Assignment 5 solution

(1) **Electron gas in 2D:** We can now routinely create materials or devices in which electron dynamics is effectively constrained to two dimensions, such as in graphene or layered semi-conductor structures.

- (a) For a gas of electrons free to move in only 2 dimensions, find the Fermi energy and temperature in terms of the 2D electron density. [5 points] *Solution: You had to adapt lecture section 4.1. from 3D to 2D. We still have occupations*

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

However when summing these up, we need to consider the reduced dimensionality

$$\Rightarrow N = \sum_{n_x, n_y, s} \bar{m}_{n_x, n_y, n_z, s} \approx \frac{2}{4} \int d^2\mathbf{n} \bar{m}_{\mathbf{n}} \quad (1)$$

$$= \frac{2\pi}{2} \int_0^{n_{max}} dn n \quad (\text{use 2D polar coordinates}) \quad (2)$$

$$= \pi \frac{n_{max}^2}{2}. \quad (3)$$

In the first equality, a factor of two is spin multiplicity, and 1/4 is due to only positive quadrant in 2D. We get  $n_{max}$  from the single particle-in-the-box energies (see appendix) as before  $n_{max} = \sqrt{\frac{2mL^2\mu}{\pi^2\hbar^2}}$ . Thus

$$N = \frac{\pi}{2} \frac{2mL^2 E_F}{\pi^2 \hbar^2} = \frac{mL^2 E_F}{\pi \hbar^2} \Rightarrow$$

$$E_F = \frac{\pi \hbar^2}{m} \underbrace{\left( \frac{N}{L^2} \right)}_{=\rho_{2D}}, \quad (4)$$

$$T_F = \frac{\pi \hbar^2 \rho_{2D}}{k_b m}. \quad (5)$$

- (b) Assume the 2D gas electrons are confined in a semi-conductor heterostructure, with the middle layer (containing the electron gas) composed of GaAs. Find or google a simple estimate for the 2D electron density in this system and use this to evaluate the quantities calculated in (a) for this system. [5 points] *Solution: The key input into any Fermi energy calculation is the free electron density. For a 3D metal, this would be easy to estimate, see e.g. [\[wikipedia on charge carrier density\]](#) using*

$$\rho_{e,3D,metal} = \frac{N_A Z n_{mass}}{m_a}, \quad (6)$$

where  $N_A$  is Avogadro's number,  $n_{mass}$  the mass density of the element,  $m_a$  its atomic mass and  $Z$  the number of valence electrons per atom.

In a 2D semi-conductor material, like GaAs, this is more complicated since it would depend on the doping and hetero-structure, hence we have to google some typical values for this material explicitly. For example in [Journal of Applied Physics \*\*123\*\*, 025302 \(2018\)](#), we can find

$$\rho_{e,2D,GaAs} = 2 \times 10^{18} \text{ m}^{-2}. \quad (7)$$

Using this value in the formulae from A gives  $E_F = 0.5 \text{ eV}$  and  $T_F = 5819 \text{ K}$ . We conclude that at room temperature (or any other temperature where the material is not destroyed), the 2D electrons in the hetero-structure form a degenerate Fermi gas. The Fermi energy is of the order of magnitude of typical band-gaps or band-widths in materials, and the precise relation of this and the structure of allowed electronic states can be important for the functioning of the material.

**(2) White dwarf stars:** Derive the maximum mass that a white dwarf star can have, assuming electrons are ultra-relativistic (energy  $\gg$  rest mass energy) and the density in the star is uniform. [10 points] *Solution:* For ultra-relativistic electrons, we can neglect the rest mass term compared to the momentum dependent term in the formula for the relativistic total energy:

$$E = \sqrt{\mathbf{p}^2 c^2 + m^2 c^4} \stackrel{v \approx c}{\approx} c|\mathbf{p}| = c\hbar|\mathbf{k}|. \quad (8)$$

If we reconsider the particle in an infinite square well potential for this case, we still can use the same wavefunctions as before, since they were determined only by the boundary-conditions and by plane-waves (or cosines/sines) being eigenfunctions of the Hamiltonian, which is still the case for our new Hamiltonian that is only a function of the momentum operator.

Placing the box from  $x = 0 \dots L$  in all three dimension, we still have allowed wavenumbers  $\mathbf{k} = [k_x, k_y, k_z]^T$  with  $k_i = n_i \pi / L$  for  $i = x, y, z$ . The modulus of the wavenumber is thus  $|\mathbf{k}| = \sqrt{n_x^2 + n_y^2 + n_z^2} \pi / L$ . Looking at energies on the Fermi energy  $E = E_F$ , Eq. (8) gives us

$$E_F = \frac{\pi c \hbar}{L} \sqrt{n_x^2 + n_y^2 + n_z^2}. \quad (9)$$

which defines a sphere in the space of quantum numbers  $\mathbf{n}$  of radius  $n_{max} = \frac{E_F L}{\pi c \hbar}$ .

As in section 4.1, we now just add occupation numbers up to the Fermi energy to express the total atom number (for Fermions with spin degeneracy  $s = 2$ ):

$$\begin{aligned} N &= 2 \sum_{\mathbf{b}} \bar{n}_{\mathbf{b}} = \sum_{n_x, n_y, n_z; |\mathbf{n}| < n_{max}} = \frac{2}{8} \int d^3_{|\mathbf{n}| < n_{max}} \mathbf{n} \\ &= \frac{4\pi}{4} \int_0^{n_{max}} dn n^2 = \frac{\pi}{3} n_{max}^3 = \frac{\pi}{3} \left( \frac{E_F L}{\pi c \hbar} \right)^3 \end{aligned} \quad (10)$$

In the third equality of the first line the factor 1/8 takes care of the fact that the original summation was over positive  $n_i$  only, while the integration contains all real values. We

can now find the Fermi energy and express the RHS in terms of the particle density in the box  $\rho = N/L^3$

$$E_F = c\hbar(3\pi^2)^{1/3} \left(\frac{N}{L^3}\right)^{1/3} = c\hbar(3\rho\pi^2)^{1/3}. \quad (11)$$

Comparing with the non-relativistic result in Eq. (4.6), the most important change is that this now scales with density as  $\rho^{1/3}$  instead of  $\rho^{2/3}$ .

We also have to modify our calculation of the degeneracy pressure, since the relation  $P \cdot V = \frac{2}{3}N\langle\varepsilon_{kin}\rangle$  used earlier does not work in the relativistic case, instead we now find the pressure using  $P = -\partial E/\partial V$ , where  $E$  is the total energy and  $V$  the volume.

To find the former:

$$\begin{aligned} E &= \frac{2}{8} \int d^3\mathbf{n} E(\mathbf{n}), \quad \left( E(\mathbf{n}) = \frac{\pi c\hbar}{L} |\mathbf{n}| \right) \\ &= \frac{4\pi}{4} \left( \frac{\pi c\hbar}{L} \right) \int_0^{n_{max}} dn n^3 \\ &= \frac{3}{4} c\hbar(3\rho/\pi)^{1/3} N = \frac{3}{4} E_F N \end{aligned}$$

The relativistic degeneracy pressure thus is

$$P_F = -\frac{\partial}{\partial V} \left( \frac{3}{4} E_F N \right) = -\frac{\partial}{\partial V} \left( \frac{3}{4} c\hbar \left( \frac{3N\pi^2}{V} \right)^{1/3} \right) N = \frac{1}{4} c\hbar \left( \frac{3N\pi^2}{V} \right)^{1/3} \frac{N}{V} = \frac{1}{4} c\hbar(3\pi^2)^{1/3} \rho^{4/3}. \quad (12)$$

This scales as  $\rho^{4/3}$  as stated in Eq. (4.14).

If we now redo the equilibrium calculation in Eq. (4.11) using this  $P_F$

$$0 = dE = \frac{\partial}{\partial R} \left( \underbrace{-\frac{3}{5} \frac{M^2}{R} G}_{E_{grav}} \right) dR \quad \underbrace{-P_F(R)(4\pi R^2 dR)}_{\text{using } dE = -PdV \text{ from thermodynamics}}. \quad (13)$$

From the mass density  $\rho_{mass} = M/(4/3\pi R^3)$ , we can infer the electron density  $2m_p\rho = \rho_{mass}$  as we did before

$$0 = \left( \frac{3GM^2}{5} - \frac{3^{5/3}\pi^{1/3}c\hbar M^{4/3}}{16m_p^{4/3}} \right) \frac{1}{R^2} \quad (14)$$

We no longer can use this to find a stable radius, since it drops out, only to know that there is no solution unless the factor in brackets vanishes, which gives us a mass

$$M = \left[ \frac{15\sqrt{5}\pi}{64} \right] \left( \frac{c\hbar}{G} \right)^{3/2} = 1.72M_\odot, \quad (15)$$

with solar mass  $M_\odot = 1.988 \times 10^{30}$  kg. The real limit is  $1.44 M_\odot$ , but for that one has to take into account the non-constant density profile of the star, so this is not too bad.

Please see pages attached at the back for much more information. Some results here disagree in numerical factors with those, please spot the mistakes and let me know. (3)

### Bosonic versus Fermionic ground-states

The template file `Assignment5_phy635_program_draft_v1.xmms` finds the ground-state of the Schrödinger equation for two Bosonic  ${}^7\text{Li}$  atoms in a one-dimensional harmonic trap using imaginary time evolution. Lithium also has a long-lived Fermionic isotope  ${}^6\text{Li}$ .

(3a) From the many-body wavefunction, derive an expression for the total density of atoms at position  $x$ . Implement the sampling of that in the last output block of the script provided. Note that the block is set up to integrate whatever is inserted over the coordinate  $x_2$ . [2 points]. *Solution: If  $\psi(x_1, x_2)$  is the manybody wavefunction of the 2 Li atoms, then total density of the atoms at some point  $x_1$  is given as:*

$$\rho(x) = 2 \int dx_2 |\psi(x, x_2)|^2 \quad (16)$$

*In general we would have that the total density is  $\rho(x) = \sum_n \rho(x_n)$ , where  $\rho(x_n)$  is the density for atom number  $n$ . We get the density for a single atom, by integrating over all other coordinates in the many-body wave function:  $\rho(x_k) = \int dx_1 dx_2 \dots \text{skip } dx_k \dots dx_N |\psi(x_1, x_2, \dots, x_k, \dots, x_N)|^2$ . Since the many-body wave function fulfills Bose symmetry all  $N$  pieces in  $\rho(x) = \sum_n \rho(x_n)$  will be identical. Hence we can just consider the density for atom one only and have  $\rho(x) = \int dx_2 \dots dx_N |\psi(x, x_2, \dots, x_k, \dots, x_N)|^2$ .*

(3b) Analytically show that the imaginary time (and real time) Schrödinger equation for two particles preserves Bosonic and Fermionic symmetries of the wave-function. [1 points] *Solution: We do this for two particles only (more follows similarly): Let us assume our wave-function fulfills  $\psi(x_1, x_2) = \pm \psi(x_2, x_1)$ . Identical particles must feel the same potential  $V(x)$  and have the same mass  $m$ , hence the SE is*

$$i\hbar \frac{\partial}{\partial t} \psi(x_1, x_2) = \left[ -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} \right) + V(x_1) + V(x_2) \right] \psi(x_1, x_2). \quad (17)$$

*We can directly see by inspection of the right-hand side that  $i\hbar \frac{\partial}{\partial t} \psi(x_1, x_2) = \pm i\hbar \frac{\partial}{\partial t} \psi(x_2, x_1)$ . Hence if the wave-function fulfills Bose or Fermi symmetry initially, it will do so at all later times as well.*

(3c) Using (4b), modify the code such that it can find the corresponding ground-state for two Fermionic atoms. Compare total densities for the Fermionic and Bosonic cases with the scripts provided. How is the Fermionic density pattern called? [3 points] *Solution: Fig. 1 is the ground state of the two-body wavefunction for the Fermions and Bosons in the harmonic trap. It is clear from the figure that time imaginary evolution preserve the Bosonic and Fermionic symmetry of the manybody wavefunction.*

(3d) Now assume the Bosons are interacting with a very short range but strong repulsive interaction  $U(x_1 - x_2) = A \exp(-\frac{|x_1 - x_2|^2}{2\sigma^2})$ . Implement that into the imaginary time evolution, and compare the ground-state and total density for the interacting

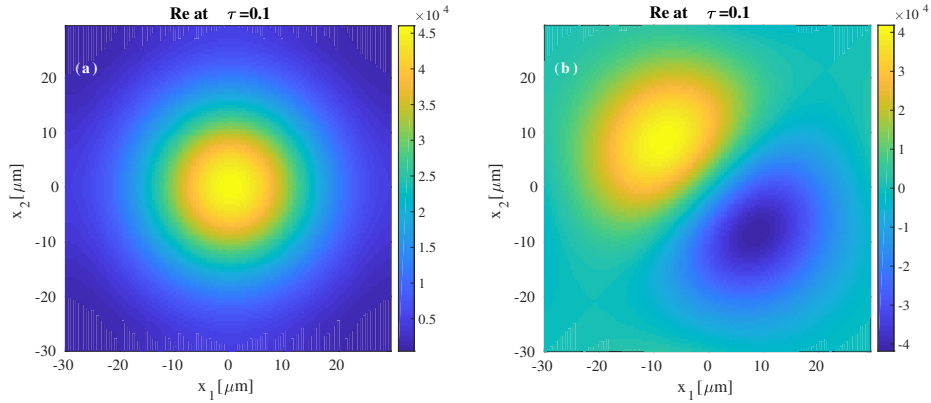


Figure 1: Panel (a) and panel (b) are the real parts of the wavefunction for Two Bosons and Fermions in the harmonic trap.

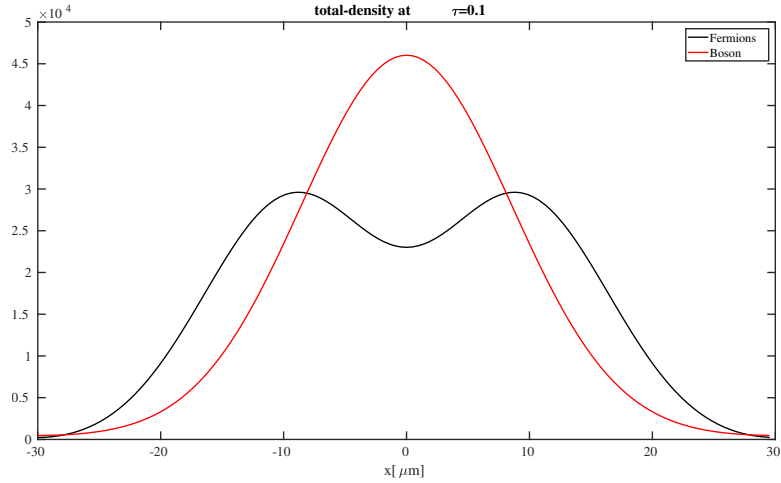


Figure 2: Comparison of the total density for two Bosons and Fermions in the harmonic trap.

Bosons, with the non-interacting **Fermions Bosons**. Discuss. [4 points] *Solution: We now add a second item into the vector potentials that we call interactions, choosing  $U(x_1 - x_2) = U_0 \exp[-(x_1 - x_2)^2 / 2\sigma_{int}^2]$ . We interpret “strong” as  $U_0 = 100\hbar\omega$  and “short range” as  $\sigma_{int} = \sigma/8$ , where  $\sigma = \sqrt{\hbar/m/\omega}$  is the harmonic oscillator ground state width. This potential essentially enforces the boundary condition  $\Psi(x_1 = x_2) = 0$  on the diagonal, due to which the Bosonic two body wavefunction looks somewhat similar to the Fermionic one, but with different signs, see Fig. 3 and compare with Fig. 1 (right). If we look at the total density instead, and compare it with the total density for the non-interacting case, see Fig. 4, we see that the repulsion somehow pushes already these two atoms outwards, as we would expect it from a GPE type of treatment. However the short range correlations due to the interactions, evident on the diagonal in Fig. 3 would not be included in the mean field treatment.*

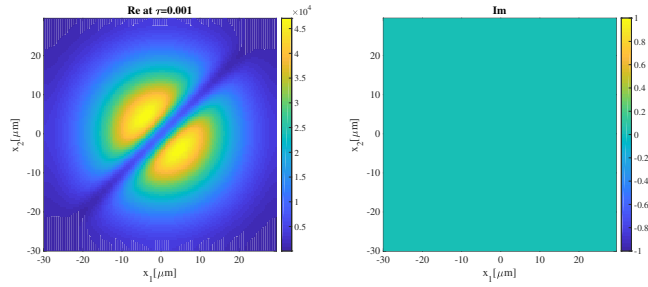


Figure 3: Bosonic ground-state wavefunction in the presence of interactions

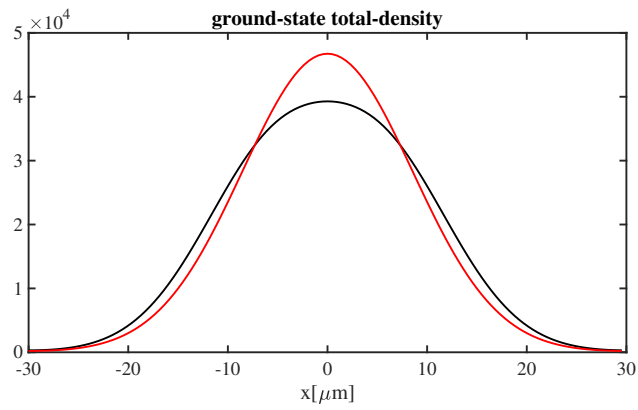


Figure 4: Comparison of total density without interactions (red) and with interactions (black)