Problem Set 6 - Fermi Gases
(Dated: PHYS403, Spring 2024)

I. Fermi Gas of ultracold ^{6}Li

Ultracold gases of fermionic atoms, such as ^{6}Li (the isotope of lithium with atomic weight 6), have been trapped and cooled with lasers to very cold temperatures below their Fermi temperature. In this question, you will numerically explore the properties of such a cold gas.

Modeling the system as an ideal free fermion gas, numerically compute and plot the chemical potential, μ, and pressure, P, for a ^{6}Li gas with average density $n = 10^{18}m^{-3}$. Plot your results for a range of T from a zero to a few times the Fermi temperature $T_F = \varepsilon_F/k_B$.

Perform your calculations in the grand-canonical ensemble. To determine μ for each temperature, T, you must (numerically) calculate the density as a function of μ and solve for the value of μ that gives the desired density, n. You may assume that each ^{6}Li atom has spin=1/2.

- μ Plot Instructions: On your plot, compute and plot a horizontal dashed line indicating the Fermi energy, ε_F, and a vertical dashed line indicating the Fermi temperature $T_F = \varepsilon_F/k_B$. Also, on the plot, plot the result for the chemical potential of a classical ideal gas. Be sure to include a legend with the curves clearly labeled.

- P Plot instructions: Plot the result in the form $PV/Nk_B = P/nk_B$ which has units of temperature (Kelvin). Also plot the same quantity for the ideal classical gas, and a horizontal dashed line for the $T = 0$ Fermi-pressure of the ideal Fermi gas. Be sure to include a legend with the curves clearly labeled.

- Include with your solution:
  1) a written note explaining/deriving any relevant quantities (you don't have to reproduce any derivations done in class or the readings, just quote the results), and
  2) a copy of the code (e.g. Jupyter notebook, python script, or mathematica workbook) that you used.

II. Doping a Semiconductor

Consider a semiconductor with conduction band $\varepsilon_{C,p} = \frac{p^2}{2m_c} + E_c$, and a valence band with energy $\varepsilon_{V,p} = -\frac{p^2}{2m} + E_V$, and band-gap of energy $E_g = E_C - E_V$.

Consider implanting a density n_d of "donor" atoms. Suppose each donor atom has a single electron orbital that can hold up to one electron, and denote the binding energy of the donor atom as ε_b.

For this problem assume that the chemical potential lies within the band-gap, and that $E_C - \mu \gg k_B T$ and $E_C - \varepsilon_b - \mu \gg k_B T$.

1. First, assume that nearly all the donors are ionized, i.e. each dopant contributes one electron to the conduction band meaning that $n_e \approx n_d$ (assuming there is a negligible population of thermal electron-hole pairs from exciting valence electrons into the conduction band). Use this expression to compute the chemical potential, μ, in terms of n_d and the conduction band parameters.

2. Now, let's evaluate the validity of our assumption. What is the probability that a dopant atom is ionized for the value of μ determined above? Under what conditions on n_d, T are we justified in assuming that almost all the donors are ionized?

3. Explain, physically, why it is possible to have a situation where $\varepsilon_b \gg k_B T$, but yet nearly all the electrons reside in the conduction band (i.e. have energy at least ε_b larger than if they were bound to a donor atom).