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FY2045 Problem set 7 fall 2023

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Problem 1

Fig. 1 shows a box with dimensions L_x and $L_y = L_z = L$, which contains a particle of mass m. One of the walls of the box is a piston which can move, so that L_x can be varied. The potential V is equal to zero inside the box and infinite outside. The energy eigenfunctions

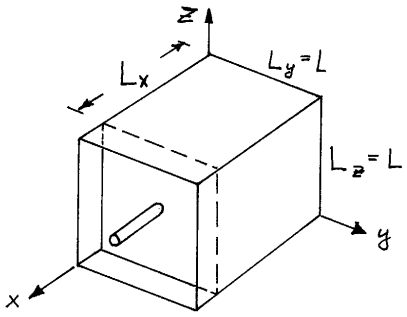

Figure 1: Box with a piston.

can be written in the form

$$\psi_{n_x,n_y,n_z} = A \sin\frac{n_x\pi x}{L_x} \sin\frac{n_y\pi y}{L} \sin\frac{n_z\pi z}{L} \ . \tag{1}$$

If the piston moves *slowly*, a particle in the state ψ_{n_x,n_y,n_z} will remain in this state, in the sense that it will keep its quantum numbers, while the wavefunction itself changes form according to the formula above, because L_x is changing. This is called an **adiabatic change** of the potential.

a) Suppose that the particle is in the ground state, show that the force on the piston exerted by the particle is

$$F_x = \frac{\hbar^2 \pi^2}{m L_x^3} \, . \tag{2}$$

Hint: Under an infinitesimal displacement dL_x of the piston, the particle does work on the piston, at the expense of the energy of the particle.

b) Suppose now that the box contains 8 non-interacting spin-$\frac{1}{2}$ particles with mass m, and that this many-particle system is in the ground state of the system, that is, has the lowest possible total energy. What is the force from the 8 particles on the piston when $L_x = L$?

Problem 2

In this problem, we are going to study the two-dimensional analog of the three-dimensional box potential discussed in class. Consider a large two-dimensional quantization area (volume) L^2. The solutions to the Schrödinger equation are products of plane waves of the form

$$\psi(x) \quad = \quad A e^{ik_x x} \, . \tag{3}$$

a) We will impose periodic boundary conditions, $\psi(0) = \psi(L)$. Find the allowed values of the momenta p_x and p_y. Use this result to find the density of states $g(p)$.

b) Assuming that the system is filled with non-interacting, identical fermions with $s = \frac{1}{2}$, calculate the particle density $\rho = N/V$, energy density $\mathcal{E} = E_{\text{tot}}/V$, and pressure P in the thermodynamic limit, i.e. for large system sizes, using the relativistic energy expression $E = \sqrt{m^2c^4 + p^2c^2}$ instead of the non-interacting gas expression $E = p^2/(2m)$ used in class.

Hint: In the thermodynamic limit we can approximate a sum over states with an integral over for instance p-space multiplied with the density of states in p-space. In class we calculated the above quantities by integrating all energies up to E_F, but in this case it might be easier to integrate all momenta $|\mathbf{p}| < p_F$.

c) Consider the ultrarelativistic ($m \to 0$) and nonrelativistic ($v = p/m \ll c$) limits and calculate the energy density and pressure. Finally, find the pressure as a function of the density.

Problem 3

(Highly voluntary — for those wanting an excuse to code.) In class, we derived the expression for the density of states for the 1D, 2D and 3D free electron gases. In this problem we will study the density of states numerically, using the definition

$$g(E) = \frac{\Delta N}{\Delta E}, \tag{4}$$

i.e. the number of energy states (ΔN) in an energy interval (ΔE).

a) Write a code that numerically calculates the density of states for the free electron gas in 3D with periodic boundary conditions. Show that it behaves in agreement with the result derived in class for low energies. Why does it not agree for high energies?

b) In class, we found that the density of states for the 2D free electron gas was constant, while in 1D and 3D it was not. Assume now that the electron energy is given by

$$E = Ak^n, \tag{5}$$

in d dimensions, where A is a constant and k is the magnitude of the wavevector $\mathbf{k}$. Make a code similar to that in a), and see if you can find combinations of n and d where the density of states is constant. Can you see a pattern?

c) In the above cases we already knew, or could calculate, the density of states analytically. However, that is not always a trivial task, in which case a numerical procedure can be a good option. This is the case with the 2D energy function

$$E(k_x, k_y) \propto -\cos k_x - \cos k_y, \tag{6}$$

which is often used to describe electrons bound more closely to the atoms in a solid (the so-called tight-binding model). Use the above numerical method to calculate the density of states for this energy function, using k-values ranging between $-\pi$ and π. Do you notice anything interesting?