

P3317 HW from Lecture 18+19 and Recitation 10

Due Nov 6, 2018

Problem 1. Equipartition *Note: This is a problem from classical statistical mechanics. We will need the answer for the next few problems, and it will reveal a failing of classical mechanics. We will then show how quantum mechanics fixes the problem.* If I wanted to challenge you I would just ask: **Find the average energy of a classical harmonic oscillator attached to a heat bath at temperature T .** That would likely cause a fit, so I've laid out the required modeling below. If you want the extra challenge, feel free to try it without looking at these hints – in that case you don't need to do all of the subparts to the problem, just come up with an answer (and give a sound argument). The answer is a famous result known as "equipartition." One of the motivators of quantum mechanics was an observed break-down of equipartition.

1.1. The first modeling step is to think of a concrete realization of a harmonic oscillator. Lets take a particle of mass m attached to a spring with spring constant $k = m\omega^2$. **Write the energy E of this particle as a function of its position x and momentum p .** [Remember, this is just classical mechanics – so its easy.]

1.2. According to classical statistical mechanics, the probability of the particle being within dx of position x and with have momentum within dp of p is

$$P(x, p) dx dp = \frac{e^{-E(x,p)/k_B T}}{Z} dx dp \quad (1)$$

where the partition function Z is a normalization constant, defined to make

$$\int P(x, p) dx dp = 1. \quad (2)$$

Write Z as an integral. You don't need to evaluate it (yet).

1.3. The average energy is then

$$\langle E \rangle = \int P(x, p) E(x, p) dx dp. \quad (3)$$

Calculate $\langle E \rangle$. Hint: its easiest if you write this as a ratio of two integrals, and make a change of variables to scale out all dimensional quantities.

You have just proved the equipartition function, which says that a classical harmonic oscillator in thermal equilibrium has energy $k_B T$, regardless of its frequency.

Problem 2. Rayleigh-Jeans Law We will use the equipartition function to estimate the spectrum of a “black body”. A black body is a model for a furnace. The idea is that inside a furnace the electromagnetic field is in thermal equilibrium with the walls. Imagine we drill a small hole in our furnace, and put a filter in the hole so that it only lets photons with an angular frequency within $d\nu$ of ν out of the hole, then the power emerging from the hole is $\Gamma(\nu)d\nu$. The function $\Gamma(\nu)$ is the *black body spectrum*.

The way we will estimate $\Gamma(\nu)$ is we will first calculate $\mathcal{I}(\nu)$, the amount of energy stored in the furnace in modes with angular frequency between ν and $\nu + d\nu$. Since all light moves at the same speed, we should have $\Gamma(\nu) \propto \mathcal{I}(\nu)$.

Recall from PHYS 2214/2218 that each mode of the electromagnetic field is just a harmonic oscillator. If we let $\rho(\nu)d\nu$ be the number of modes in the cavity with angular frequency within $d\nu$ of ν , then equipartition tells us that the energy contained in those modes will be

$$\mathcal{I}(\nu)d\nu = k_B T \rho(\nu)d\nu. \quad (4)$$

The function $\rho(\nu)$ is known as the density of states.

2.1. To find the electromagnetic modes in the furnace, we would in principle need to know all sorts of details about its shape and the material properties. (For example, conducting walls will give different boundary conditions for Maxwell’s equations than insulating walls.) We just need an estimate though, so we will treat the furnace as a cubic box of length L , with periodic boundary conditions. You can also use “hard wall” boundary conditions if you prefer. The result is the same in the end.

What are the allowed wavevectors for electromagnetic waves in a box of length L ?

2.2. Write a sum which expresses how many modes have angular frequency less than ν . Call this quantity $\mathcal{N}(\nu)$. [This is similar to the calculation you did in the homework problem on Fermi Pressure, except the dispersion is different.] Ignore polarization.

2.3. Approximate the sum as an integral, and perform the integral to estimate $\mathcal{N}(\nu)$.

2.4. The number of modes is just the integral of the density of states:

$$\mathcal{N}(\nu) = \int_0^\nu \rho(\bar{\nu}) d\bar{\nu}. \quad (5)$$

Take a derivative to calculate $\rho(\nu)$.

2.5. How does $\Gamma(\nu)$ scale with ν for larger ν . This is known as the Rayleigh-Jeans law.

If you actually do the experiment, you will see that $\Gamma(\nu) \rightarrow 0$ as $\nu \rightarrow \infty$. Thus the classical theory gives a qualitatively incorrect result.

Problem 3. Energy in a Thermal Quantum Harmonic Oscillator

The error in Rayleigh and Jeans' argument is that equipartition does not hold in a quantum world. The eigenstates of the harmonic oscillator are labeled by an integer n . The average energy at temperature T should be

$$\langle E \rangle = \frac{\sum_n E_n e^{-E_n/k_B T}}{Z}, \quad (6)$$

where

$$Z = \sum_n e^{-E_n/k_B T}. \quad (7)$$

3.1. Calculate Eq. (6), using the spectrum of a harmonic oscillator. Do not include the zero-point energy, as it will not contribute to the power emerging from the furnace. That is take $E_n = \hbar\omega n$ for integer n .

3.2. Under what circumstances does this reduce to the classical equipartition result?

Problem 4. Planck

4.1. How should equation (4) be corrected to account for the quantum mechanical result you found in problem 3?

4.2. What is the quantum result for $\Gamma(\nu)$ – this is known as the Planck black body spectrum. Don't worry about multiplicative constants, I just want to know how it scales with ν .

4.3. How does $\Gamma(\nu)$ behave as $\nu \rightarrow \infty$?

4.4. Plot $\Gamma(\nu)$. Label your graph (you may use "arbitrary units" for the vertical axis, but on the horizontal axis, locate the point where $\hbar\nu = k_B T$).

Problem 5. Two coupled oscillators

To help you with this problem I will give another quick review of ladder operators. We begin with the simple harmonic oscillator (in dimensionless coordinates):

$$\hat{H} = \frac{1}{2}\hat{p}^2 + \frac{1}{2}\hat{x}^2. \quad (8)$$

One then defines $\hat{a} = (\hat{x} + i\hat{p})/\sqrt{2}$ and $\hat{a}^\dagger = (\hat{x} - i\hat{p})/\sqrt{2}$, which explicitly obey $[\hat{a}, \hat{a}^\dagger] = 1$. In terms of these operators, one can write

$$\hat{H} = \hat{a}^\dagger \hat{a} + \frac{1}{2}. \quad (9)$$

Using our favorite identity $[A, BC] = B[A, C] + [A, B]C$, we immediately see $[\hat{a}, \hat{H}] = a$ and $[\hat{a}^\dagger, \hat{H}] = -a^\dagger$. This instantly gives us a ladder of states. We start by defining $\psi_0(x)$ to be the wavefunction obeying

$$\hat{a}\psi_0(x) = 0. \quad (10)$$

This is a 1st order differential equation, and easy to solve (the answer is a Gaussian). Clearly

$$\hat{H}\psi_0 = \frac{1}{2}\psi_0. \quad (11)$$

We now get a ladder of states. Not worrying about normalization, we define

$$\psi_j = a^\dagger \psi_{j-1}. \quad (12)$$

If ψ_{j-1} is an eigenstate of H with eigenvalue E_{j-1} , we find

$$H\psi_j = H a^\dagger \psi_{j-1} = (a^\dagger H + a^\dagger) \psi_{j-1} = (E_{j-1} + 1) a^\dagger \psi_{j-1} = (E_{j-1} + 1) \psi_j, \quad (13)$$

which tells us that ψ_j is also an eigenstate, and the energies form a ladder: $E_j = j + 1/2$.

In class we have been looking at a problem with coupled oscillators. We were thinking about a long chain, but in this problem we will consider just two oscillators:

$$\hat{H} = \frac{1}{2}(\hat{p}_1^2 + \hat{p}_2^2) + \frac{1}{2}(\hat{x}_1^2 + \hat{x}_2^2) + \alpha(x_1 - x_2)^2. \quad (14)$$

Using the argument in class we can define operators \hat{a}_1 and \hat{a}_2 which obey $[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij}$ and $[\hat{a}_i, \hat{a}_j] = 0$. The expressions for these operators are kind of ugly, but the end result (that we spent quite some time proving) is that

$$\hat{H} = A + \epsilon \left(\hat{a}_1^\dagger \hat{a}_1 + \hat{a}_2^\dagger \hat{a}_2 \right) - J \left(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1 \right), \quad (15)$$

where A, ϵ, J are all functions of α . In this question we will explore the properties of Eq. (15).

5.1. Define a wavefunction $\psi_{00}(x_1, x_2)$ such that

$$\hat{a}_1 \psi_{00} = 0 \quad (16)$$

$$\hat{a}_2 \psi_{00} = 0. \quad (17)$$

This is known as “the vacuum state”. It is the state with no phonons. It is the natural generalization of Eq. (10).

Prove that ψ_{00} is an eigenstate of \hat{H} . What is the eigenvalue?

5.2. We define a normalized wavefunction ψ_{nm} as

$$\psi_{nm} = \frac{1}{\sqrt{n!m!}} \left(a_1^\dagger\right)^n \left(a_2^\dagger\right)^m \psi_{00}. \quad (18)$$

Is ψ_{10} an eigenstate of \hat{H} ? If so, what is the eigenvalue.

5.3. Consider a wavefunction

$$\psi(x_1, x_2, t) = a(t)\psi_{1,0}(x_1, x_2) + b(t)\psi_{0,1}(x_1, x_2). \quad (19)$$

This is the most general wavefunction in the “one phonon sector”. The coefficient $|a|^2$ is interpreted as the probability of the phonon being on the first oscillator, and $|b|^2$ is the probability it is on the second oscillator.

From the time dependent Schrodinger equation $i\partial_t\psi = \hat{H}\psi$, find a differential equation for $a(t)$ and $b(t)$.

Your result should be reminiscent of your model for Ammonia: The equations of motion for a phonon in these two coupled oscillators is identical to the equation of motion for a particle in a double well.

5.4. The operator which measures the total number of phonons is $\hat{N} = \hat{a}_1^\dagger\hat{a}_1 + \hat{a}_2^\dagger\hat{a}_2$. Show that $[\hat{N}, \hat{H}] = 0$, which means that the number of phonons is conserved.

Problem 6. Magnons

In class we studied a model of phonons: quanta of vibration in coupled mechanical systems. Here you will do a similar thing with excitations of a set of coupled spins. This is actually a simpler model. These quanta of excitations are typically called Magnons. [Note, they are not called spinons – spinons are something else.]

There are a number of molecules which can be thought of as spin chains, for example we can consider a polymer made of CsFeBr₃. The iron is magnetic – meaning it has a net spin. It turns out in this context the spin is 1.

Spin 1 chains are really interesting, but we will save that for another day – here we will think about the spin-1/2 chain. We imagine we have n sites in a line. At each site there is a spin-1/2. The Hilbert space is spanned by states like $|\uparrow\uparrow\downarrow\uparrow\downarrow\cdots\rangle$, where we specify the spin on each site. We are

going to start with a state $|j\rangle$ where all of the spins are down except the j 'th spin, and ask how the Hamiltonian acts on that state.

The strongest interaction will be among neighboring spins. Assuming nothing is breaking rotational invariance, we expect a Hamiltonian something like

$$H = -J \sum_{i=1}^{n-1} \mathbf{S}_i \cdot \mathbf{S}_{i+1}. \quad (20)$$

[This is known as the Heisenberg model of a spin chain. Other models include “Ising, XY, XXZ, XYZ” which are similar, but have some rotational anisotropy.] We will assume that the coefficient J is positive, which means neighboring spins want to point in the same direction. This is a model of a ferromagnet. The ground state has all of the spins aligned.

Recall, that \mathbf{S} represents the vector of operators $\mathbf{S} = (S_x, S_y, S_z)$, with $S_x = (S_+ + S_-)/2$, and $S_y = (S_+ - S_-)/(2i)$.

- 6.1.** Write $\mathbf{S}_i \cdot \mathbf{S}_{i+1}$ in terms of $S_i^z, S_i^+, S_i^-, S_{i+1}^z, S_{i+1}^+, S_{i+1}^-$.
- 6.2.** Argue that $H|j\rangle$ is a linear superposition of states $|j\rangle, |j+1\rangle$ and $|j-1\rangle$. Find the coefficients.
- 6.3.** Your last result shows that the states $|1\rangle, |2\rangle, \dots, |n\rangle$ are closed under the action of H . Write the matrix representation of H in this space.

You can identify your matrix as the finite difference approximation to the Hamiltonian for a particle. Thus the excitations of the spin chain act like quantum mechanical particles, and obey the single particle Schrodinger equation. Single particle quantum mechanics *emerges* as an effective model of the excitations of a spin chain.

Problem 7. Feedback

- 7.1.** How long did this homework take?
- 7.2.** Which of the following words come to mind when you think about this homework (feel free to add your own words if you have something better): frustrating, fun, tedious, insightful, hard, easy, useful, useless, fair, unfair