

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.]

Solution 1.1 (1 point).

$$E = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2x^2 \quad (1)$$

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

$$P(x, p) dx dp = \frac{e^{-E(x,p)/k_B T}}{Z} dx dp \quad (2)$$

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

$$\int P(x, p) dx dp = 1. \quad (3)$$

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

Solution 1.2 (2 points). Since

$$\int P(x, p) dx dp = \frac{1}{Z} \int e^{-E(x,p)/k_B T} dx dp = 1, \quad (4)$$

this implies that

$$Z = \int e^{-\beta(\frac{1}{2m}p^2 + \frac{1}{2}m\omega^2x^2)} dx dp \quad (5)$$

1.3. The average energy is then

$$\langle E \rangle = \int P(x, p) E(x, p) dx dp. \quad (6)$$

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.

Solution 1.3 (2 points). Following the suggestion of the question, we write

$$\langle E \rangle = \frac{\int e^{-\beta(\frac{1}{2m}p^2 + \frac{1}{2}m\omega^2x^2)} (\frac{1}{2m}p^2 + \frac{1}{2}m\omega^2x^2) dx dp}{\int e^{-\beta(\frac{1}{2m}p^2 + \frac{1}{2}m\omega^2x^2)} dx dp}. \quad (7)$$

We then rescale the variables, letting $y = (\beta m \omega^2 / 2)^{1/2} x$, and $k = (\beta / 2m)^{1/2} p$, to find

$$\langle E \rangle = \frac{1}{\beta} \frac{\int e^{-y^2 - k^2} (y^2 + k^2) dy dk}{\int e^{-y^2 - k^2} dy dk} \quad (8)$$

$$= \frac{1}{\beta} \left[\frac{\int e^{-y^2} y^2 dy}{\int e^{-y^2} dy} + \frac{\int e^{-k^2} k^2 dy}{\int e^{-k^2} dk} \right] \quad (9)$$

$$= \frac{2}{\beta} \frac{\int e^{-y^2} y^2 dy}{\int e^{-y^2} dy} \quad (10)$$

$$= \frac{1}{\beta}, \quad (11)$$

where we used the Gaussian integral formulas from Homework 1. There are, of course a few other equally good tricks for doing this.

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

$$\mathcal{I}(\nu)d\nu = k_B T \rho(\nu)d\nu. \quad (12)$$

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 ?

Solution 2.1 (2 points). Periodicity implies

$$e^{ik_x x} = e^{ik_x(x+L)} \quad (13)$$

and so $k_x = \frac{2\pi}{L}n_x$ for $n_x \in \mathbb{Z}$. By the same argument $k_y = \frac{2\pi}{L}n_y$ and $k_z = \frac{2\pi}{L}n_z$.

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.

Solution 2.2 (2 points). Since $\omega = c|\vec{k}|$, if we want modes with ω less than ν , this is equivalent to finding the 3-tuples (n_x, n_y, n_z) such that

$$\frac{2\pi c}{L} \sqrt{n_x^2 + n_y^2 + n_z^2} < \nu \quad (14)$$

Ignoring photon polarisation, we just sum over all such 3-tuples that satisfy the inequality above to get the total number of modes.

$$N(\nu) = \sum_{n_x, n_y, n_z \in \mathbb{Z}, \sqrt{n_x^2 + n_y^2 + n_z^2} < \frac{L\nu}{2\pi c}} 1 \quad (15)$$

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

Solution 2.3 (2 points). Just as we did in Homework 7, we can approximate this sum as an integral. Define $R = \frac{L\nu}{2\pi c}$.

$$N(\nu) = \int_{n_x^2 + n_y^2 + n_z^2 < R^2} dn_x dn_y dn_z = \frac{4}{3}\pi R^3 = \frac{L^3 \nu^3}{6\pi^2 c^3} \quad (16)$$

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

$$\mathcal{N}(\nu) = \int_0^\nu \rho(\bar{\nu}) d\bar{\nu}. \quad (17)$$

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

Solution 2.4 (2 points).

$$\rho(\nu) = \frac{\partial \mathcal{N}(\nu)}{\partial \nu} = \frac{L^3 \nu^2}{2\pi^2 c^3} \quad (18)$$

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

Solution 2.5 (2 points). Since $\Gamma(\nu) \propto \mathcal{I}(\nu) \propto k_B T \rho(\nu)$, we expect $\Gamma(\nu) \propto \nu^2$. So $\Gamma(\nu)$ should scale quadratically with ν .

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

$$\langle E \rangle = \frac{\sum_n E_n e^{-E_n/k_B T}}{Z}, \quad (19)$$

where

$$Z = \sum_n e^{-E_n/k_B T}. \quad (20)$$

3.1. Calculate Eq. (19), 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 .

Solution 3.1 (3 points). Ignoring ground state energy,

$$\begin{aligned}
 Z &= \sum_{n=0}^{\infty} e^{-\hbar\omega n\beta} \\
 &= \sum_{n=0}^{\infty} e^{-\hbar\omega n\beta} \\
 &= \frac{1}{1 - e^{-\hbar\omega\beta}}
 \end{aligned} \tag{21}$$

where in the last step we have evaluated the sum by recognizing that it is a geometric series. One slick way to calculate the energy is to note that

$$\begin{aligned}
 \langle E \rangle &= -\frac{1}{Z} \frac{\partial Z}{\partial \beta} \\
 &= -\frac{1}{Z} \left[\frac{-(-\hbar\omega)(-e^{-\hbar\omega\beta})}{(1 - e^{-\hbar\omega\beta})^2} \right] \\
 &= \frac{\hbar\omega e^{-\hbar\omega\beta}}{1 - e^{-\hbar\omega\beta}} \\
 &= \frac{\hbar\omega}{e^{\hbar\omega\beta} - 1}.
 \end{aligned} \tag{22}$$

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

Solution 3.2 (1 point). We get the classical equipartition result if $\hbar\omega\beta \ll 1$, or $k_B T \gg \hbar\omega$.

Problem 4. Planck

4.1. How should equation (12) be corrected to account for the quantum mechanical result you found in problem 3?

Solution 4.1 (2 points). Since the equipartition theorem no longer holds, we should replace the $k_B T$ factor in

$$I(\nu)d\nu = k_B T \rho(\nu)d\nu \tag{23}$$

by our results for $\langle E \rangle$:

$$I(\nu)d\nu = \frac{\hbar\nu}{e^{\hbar\nu\beta} - 1} \rho(\nu)d\nu \tag{24}$$

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 .

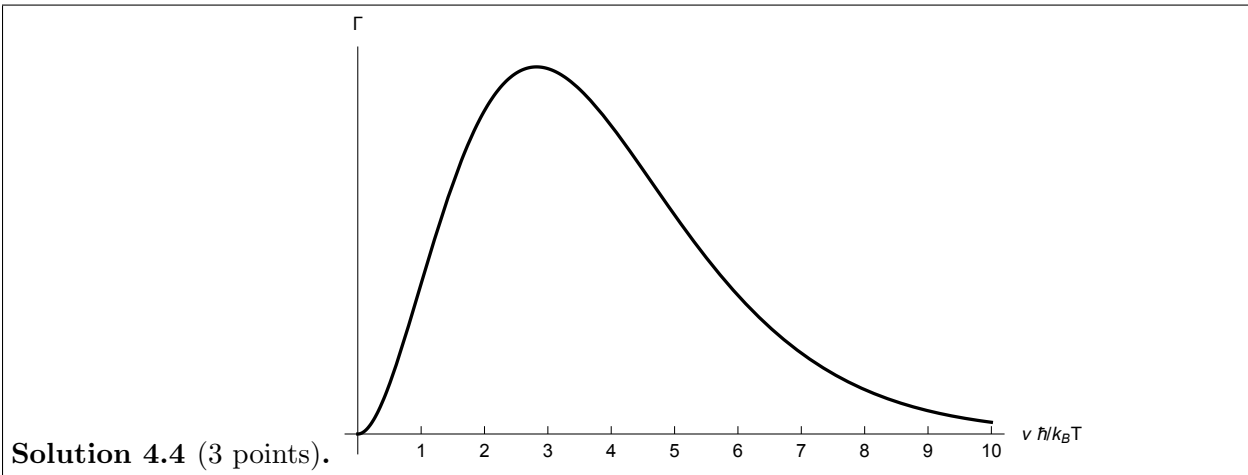
Solution 4.2 (3 points). Recalling our results for $\rho(\nu)$ earlier on,

$$\begin{aligned}
 \Gamma(\nu) &\propto I(\nu) \\
 &= \frac{\hbar\nu}{e^{\hbar\nu\beta} - 1} \rho(\nu) \\
 &= \frac{\hbar\nu}{e^{\hbar\nu\beta} - 1} \frac{L^3\nu^2}{2\pi^2c^3} \\
 &= \frac{\hbar L^3}{2\pi^2c^3} \frac{\nu^3}{e^{\hbar\nu\beta} - 1} \\
 &\propto \frac{\nu^3}{e^{\hbar\nu\beta} - 1}
 \end{aligned} \tag{25}$$

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

Solution 4.3 (1 point). As $\nu \rightarrow \infty$, $\frac{1}{e^{\hbar\nu\beta} - 1} \sim e^{-\hbar\nu\beta}$, which overwhelms the ν^3 factor. Therefore, $\Gamma(\nu)$ exponentially decays to zero.

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):

$$\hat{H} = \frac{1}{2}\hat{p}^2 + \frac{1}{2}\hat{x}^2. \quad (26)$$

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

$$\hat{H} = \hat{a}^\dagger \hat{a} + \frac{1}{2}. \quad (27)$$

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

$$\hat{a}\psi_0(x) = 0. \quad (28)$$

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

$$\hat{H}\psi_0 = \frac{1}{2}\psi_0. \quad (29)$$

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

$$\psi_j = \hat{a}^\dagger \psi_{j-1}. \quad (30)$$

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

$$H\psi_j = H\hat{a}^\dagger\psi_{j-1} = (\hat{a}^\dagger H + \hat{a}^\dagger)\psi_{j-1} = (E_{j-1} + 1)\hat{a}^\dagger\psi_{j-1} = (E_{j-1} + 1)\psi_j, \quad (31)$$

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:

$$\hat{H} = \frac{1}{2}(\hat{p}_1^2 + \hat{p}_2^2) + \frac{1}{2}(\hat{x}_1^2 + \hat{x}_2^2) + \alpha(x_1 - x_2)^2. \quad (32)$$

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

$$\hat{H} = A + \epsilon \left(\hat{a}_1^\dagger \hat{a}_1 + \hat{a}_2^\dagger \hat{a}_2 \right) - J \left(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1 \right), \quad (33)$$

where A, ϵ, J are all functions of α . In this question we will explore the properties of Eq. (33).

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

$$\hat{a}_1 \psi_{00} = 0 \quad (34)$$

$$\hat{a}_2 \psi_{00} = 0. \quad (35)$$

This is known as “the vacuum state”. It is the state with no phonons. It is the natural generalization of Eq. (28).

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

Solution 5.1 (2 points).

$$\hat{H}\psi_{00} = \left[A + \epsilon \left(\hat{a}_1^\dagger \hat{a}_1 + \hat{a}_2^\dagger \hat{a}_2 \right) - J \left(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1 \right) \right] \psi_{00} \quad (36)$$

$$= A\psi_{00} + \epsilon \hat{a}_1^\dagger \hat{a}_1 \psi_{00} + \epsilon \hat{a}_2^\dagger \hat{a}_2 \psi_{00} - J \hat{a}_1^\dagger \hat{a}_2 \psi_{00} - J \hat{a}_2^\dagger \hat{a}_1 \psi_{00} \quad (37)$$

$$= A\psi_{00} \quad (38)$$

This means that ψ_{00} is an eigenstate of \hat{H} , with eigenvalue A .

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

$$\psi_{nm} = \frac{1}{\sqrt{n!m!}} \left(a_1^\dagger \right)^n \left(a_2^\dagger \right)^m \psi_{00}. \quad (39)$$

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

Solution 5.2 (3 points).

$$\psi_{10} = a_1^\dagger \psi_{00}. \quad (40)$$

We will want to see if $\hat{H}\psi_{10} = \lambda\psi_{10}$ for some λ . Before jumping in, note that:

$$\hat{a}_1 \psi_{10} = a_1 a_1^\dagger \psi_{00} = \left(1 + a_1^\dagger a_1 \right) \psi_{00} = \psi_{00} \quad (41)$$

$$\hat{a}_2 \psi_{10} = a_2 a_1^\dagger \psi_{00} = a_1^\dagger a_2 \psi_{00} = 0. \quad (42)$$

Now:

$$\hat{H}\psi_{10} = A\psi_{10} + \epsilon \hat{a}_1^\dagger \hat{a}_1 \psi_{10} + \epsilon \hat{a}_2^\dagger \hat{a}_2 \psi_{10} - J \hat{a}_1^\dagger \hat{a}_2 \psi_{10} - J \hat{a}_2^\dagger \hat{a}_1 \psi_{10} \quad (43)$$

$$= (A + \epsilon) \psi_{10} - J \hat{a}_2^\dagger \psi_{00} \quad (44)$$

$$= (A + \epsilon) \psi_{10} - J \psi_{01}. \quad (45)$$

ψ_{10} is therefore not an eigenstate of the Hamiltonian: a particle initially in state ψ_{10} will evolve in to a linear combination of ψ_{01} and ψ_{10} .

5.3. Consider a wavefunction

$$\psi(x_1, x_2, t) = a(t)\psi_{1,0}(x_1, x_2) + b(t)\psi_{0,1}(x_1, x_2). \quad (46)$$

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.

Solution 5.3 (3 points).

$$i\partial_t\psi = \hat{H}\psi \quad (47)$$

$$= a(t)\hat{H}\psi_{10} + b(t)\hat{H}\psi_{01}. \quad (48)$$

We found $\hat{H}\psi_{10}$ already. By symmetry, we can see that $\hat{H}\psi_{01}$ is the same as the expression for ψ_{10} but with the labels 1 and 0 swapped:

$$\hat{H}\psi_{01} = (A + \epsilon)\psi_{01} - J\psi_{10}. \quad (49)$$

Therefore:

$$i\partial_t\psi = \hat{H}\psi \quad (50)$$

$$= [a(t)(A + \epsilon) - Jb(t)]\psi_{10} + [b(t)(A + \epsilon) - Ja(t)]\psi_{01}. \quad (51)$$

By isolating coefficients for ψ_{10} and ψ_{01} , we can extract the two first-order differential equations:

$$i\hbar\partial_t a(t) = (A + \epsilon)a(t) - Jb(t) \quad (52)$$

$$i\hbar\partial_t b(t) = (A + \epsilon)b(t) - Ja(t). \quad (53)$$

The simplest way to solve this, as with the ammonia molecule, is to find the eigenvectors and eigenvalues of the Hamiltonian matrix.

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.

Solution 5.4 (2 points). Let me write the Hamiltonian in four terms:

$$\hat{H} = A + \epsilon\hat{N} - J \left(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1 \right). \quad (54)$$

Clearly \hat{N} commutes with the first two terms, so let us focus on the last two:

$$\left[\hat{N}, \hat{a}_1^\dagger \hat{a}_2 \right] = \left[\hat{N}_1, a_1^\dagger a_2 \right] + \left[\hat{N}_2, a_1^\dagger a_2 \right] \quad (55)$$

$$= a_1^\dagger a_2 - a_1^\dagger a_2 \quad (56)$$

$$= 0. \quad (57)$$

This is because the operator $\hat{a}_1^\dagger \hat{a}_2$ increases particle number 1 by one, and decreases particle number 2 by one, so that the sum of the two particle numbers is conserved. Similarly for the last term. Therefore, $\left[\hat{N}, \hat{H} \right] = 0$.

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 $|\uparrow\uparrow\downarrow\uparrow\downarrow \dots\rangle$, 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

$$H = -J \sum_{i=1}^{n-1} \mathbf{S}_i \cdot \mathbf{S}_{i+1}. \quad (58)$$

[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 $S_i^z, S_i^+, S_i^-, S_{i+1}^z, S_{i+1}^+, S_{i+1}^-$.

Solution 6.1 (2 points).

$$\mathbf{S}_i \cdot \mathbf{S}_{i+1} = S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z. \quad (59)$$

Now, recall that:

$$S^x = (S^+ + S^-) / 2 \quad (60)$$

$$S^y = -i (S^+ - S^-) / 2. \quad (61)$$

It may be more intuitive to think about the matrix representations:

$$S^x = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad S^y = \frac{1}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad (62)$$

$$S^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad S^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \quad (63)$$

It follows that:

$$\mathbf{S}_i \cdot \mathbf{S}_{i+1} = \frac{1}{4} (S_i^+ S_{i+1}^+ + S_i^- S_{i+1}^- + S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) \quad (64)$$

$$\begin{aligned} & - \frac{1}{4} (S_i^+ S_{i+1}^+ + S_i^- S_{i+1}^- - S_i^+ S_{i+1}^- - S_i^- S_{i+1}^+) + S_i^z S_{i+1}^z \\ & = \frac{1}{2} (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) + S_i^z S_{i+1}^z \end{aligned} \quad (65)$$

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.

Solution 6.2 (3 points). The terms in the operator $(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) / 2$ raises the spin on one site and lowers the spin on a neighbouring site. It will therefore destroy a state when it acts on two neighbouring sites with the same spin. In other words

$$\frac{1}{2} \sum_i (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) |j\rangle = \frac{1}{2} (S_{j-1}^+ S_j^- + S_j^- S_{j+1}^+) |j\rangle = \frac{|j+1\rangle + |j-1\rangle}{2}, \quad (66)$$

and so this part of the Hamiltonian lowers the spin on site j , while raising it on the neighbouring sites. The part of the Hamiltonian given by $\sum_i S_i^z S_{i+1}^z$ will change the state only by a multiplicative constant, since all of the sites are in eigenstates of the S^z operator. To figure out what this multiplicative constant will be, note that $S_i^z S_{i+1}^z = 1/4$ if both spins i and $i+1$ are in the same direction, and $S_i^z S_{i+1}^z = -1/4$ if the two spins are in opposite directions. Therefore, $\sum_i S_i^z S_{i+1}^z |j\rangle = (n-3)/4 - 2/4$, and:

$$H |j\rangle = -J \sum_{i=1}^{n-1} \mathbf{S}_i \cdot \mathbf{S}_{i+1} |j\rangle = -\frac{J}{2} (|j+1\rangle + |j-1\rangle) - J \frac{n-5}{4} |j\rangle \quad (67)$$

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.

Solution 6.3 (3 points). Writing the state vector for a generic ‘one-particle’ state $|\psi\rangle = \sum_i c_i |i\rangle$, or as a column vector:

$$|\psi\rangle = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix}, \quad (68)$$

the Hamiltonian becomes:

$$H = -\frac{J}{4} \begin{pmatrix} n-5 & 2 & 0 & 0 & & \\ 2 & n-5 & 2 & 0 & \dots & \\ 0 & 2 & n-5 & 2 & & \\ 0 & 0 & 2 & n-5 & & \\ & \vdots & & & \ddots & \end{pmatrix}. \quad (69)$$

An upward-pointing spin will travel backwards and forwards along the spin-chain like a free particle moving in one dimension. ‘Really’, the particles are the stationary sites, and their spins are behaving collectively. But this collective motion of spins has all the properties of a particle: it has a mass, a momentum, quantized energy. It is most usefully thought of as a particle.

One take-away is that we can think of all particles as perhaps just being excitations of some fields. This is the interpretation most commonly used in high energy physics.

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