UCSB, Physics 129AL, Computational Physics: Section Worksheet, Week 6A

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Section Participation and Submission Guidelines

Section attendance is required, but you do not need to complete all the work during the section. At each section, the TA will answer any questions that you might have, and you are encouraged to work with others and look for online resources during the section and outside of sections. Unless otherwise stated, the work will be due one week from the time of assignment. The TA will give you 1 point for each task completed. You can see your grades on Canvas.

We will use GitHub for section worksheet submissions. By the due date, you should have a single public repository on GitHub containing all the work you have done for the section work. Finally, upload a screenshot or a .txt file to Canvas with your GitHub username and repository name so the TA knows who you are and which repository you are using for the section.

Remember: talk to your fellow students, work together, and use GPTs. You will find it much easier than working alone. Good luck! All work should be done in the Docker container, and don't forget to commit it to Git!

Task 1: Poisson

Consider an example in astrophysics. Let's assume stars randomly distributed around us with density n, what is probability that the nearest star is at distance R ?

Task 2: Lorentzian

Resonance behavior is critical for understanding the energy dissipation and absorption of a system. Let's consider a general dissipative, driven harmonic oscillator in both time and frequency domain,

$$\frac{\mathrm{d}^2x}{\mathrm{d}t^2} + \gamma\frac{\mathrm{d}x}{\mathrm{d}t} + \omega_0^2 x = Fe^{i\omega_f t}, \quad -\omega^2\tilde{x} + i\gamma\omega\tilde{x} + \omega_0^2\tilde{x} = F\delta(\omega - \omega_f), \tag{1}$$

where $\tilde{x}$ and x are related via Fourier transform. Show that the energy absorption per cycle is a Lorentzian,

$$E = F\pi \frac{\gamma\omega_f}{(\omega_0^2 - \omega_f^2)^2 + \gamma^2\omega_f^2}. \tag{2}$$

Hint: $\sin(\Sigma) = -A\gamma\omega_f$.

Task 2: Revisit the Heisenberg XXX Hamiltonian on a Ring: Markov Chain

In the previous section, we have looked at the Heisenberg XXX Hamiltonian spectrum on a ring using various matrix techniques. In this task, you are asked to construct the Markov chain that simulate

Let us introduce the raising and lowering operators $S_\pm = S_x \pm iS_y$, such that

$$S_+|\uparrow\rangle = 0, \quad S_-|\uparrow\rangle = |\downarrow\rangle, \quad S_z|\uparrow\rangle = \frac{1}{2}|\uparrow\rangle$$
$$S_+|\downarrow\rangle = |\uparrow\rangle, \quad S_-|\downarrow\rangle = 0, \quad S_z|\downarrow\rangle = -\frac{1}{2}|\downarrow\rangle. \tag{4}$$

We can write the XXX Hamiltonian as the following,

$$H = \frac{JN}{4} - J\sum_{i=1}^{N} \frac{1}{2}\left(S_{+i}S_{-i+1} + S_{-i}S_{+i+1}\right) + S_{zi}S_{zi+1}, \tag{5}$$

with periodic boundary condition, such that $N + 1 = 1$.

Let us look at the different terms. The terms involving $S_\pm$ are called hopping terms since they move a spin up or spin down to a neighboring site. The constant term proportional to N is added for convenience. It is simply an overall shift of the energy levels. Depending on the sign, you want to align or anti-align the spins, i.e. (anti-)ferromagnetism.

The above Hamiltonian can be written in a matrix form with a given Hilbert space. let's consider a simple 3-spin chain, where the index location represents the sites, i.e. $1, 2, 3$. The Hamiltonian for the Heisenberg XXX model with $N = 3$ spins is given by,

$$H = \frac{3J}{4} - J\left[\frac{1}{2}\left(S_{+1}S_{-2} + S_{-1}S_{+2}\right) + S_{z1}S_{z2} + \frac{1}{2}\left(S_{+2}S_{-3} + S_{-2}S_{+3}\right) + S_{z2}S_{z3} + \frac{1}{2}\left(S_{+3}S_{-1} + S_{-3}S_{+1}\right) + S_{z3}S_{z1}\right]$$

with states,

$$(|\uparrow\uparrow\uparrow\rangle, |\uparrow\uparrow\downarrow\rangle, |\uparrow\downarrow\uparrow\rangle, |\uparrow\downarrow\downarrow\rangle, |\downarrow\uparrow\uparrow\rangle, |\downarrow\uparrow\downarrow\rangle, |\downarrow\downarrow\uparrow\rangle, |\downarrow\downarrow\downarrow\rangle).$$

The corresponding marginal distribution is given by,

$$\pi = (\pi_1, \pi_2, \cdots, \pi_8). \tag{3}$$

For example, matrix element can be calculate via the following expression,

$$\langle\downarrow\uparrow\downarrow| S_{+2}S_{-3}|\downarrow\downarrow\uparrow\rangle = 1. \tag{4}$$

Question 1: Markov chain in site basis

Using the above Hamiltonian, construct the Markov chain for the above $N = 3$ system. What are the transition probabilities? Write it in a matrix form.

Question 2: Markov chain in site basis

At a given temperature, find a stationary distribution π by solving the following expression,

$$\pi P = \pi, \quad \text{and} \quad \sum_{i=1}^{k} \pi_i = 1.$$

Question 3: Markov chain in site basis

Use the power iteration,

$$\pi_{k+1} = \pi_k P$$

, to find the stationary distribution for the following three initial guesses,

- 1) $\Pr(|\uparrow\uparrow\uparrow\rangle) = 1$,
- 2) $\Pr(|\uparrow\uparrow\uparrow\rangle) = \frac{1}{2}, \Pr(|\downarrow\uparrow\downarrow\rangle) = \frac{1}{2}$,
- 3) a uniformly distributed initial configuration.

Question 4: Markov chain in magnon basis

Let's say we are only interested in the population probabilities (diagonal term in the density matrix) of magnons, where we can model the transition between magnons $|k\rangle \to |k'\rangle$ classically via the **classical master equation**. We should note that if the off-diagonal terms are large (represents the coherence than number statistics), we must use the quantum master equation (Lindblad master equation).

Recall the magnon formulation: **Ground state.** Since the total spin is conserved, the state in which all spins are aligned in the same direction must be an eigenstate of the Hamiltonian. This corresponds to the ferromagnetic vacuum. Therefore, we define the vacuum state as

$$|0\rangle = |\uparrow\uparrow\ldots\uparrow\rangle.$$

It is straightforward to calculate the energy of this state:

$$H|0\rangle = 0.$$

The **magnon (spin wave) state** is defined as:

$$|p\rangle = \sum_n e^{ipn} S_{-n} |0\rangle$$

where i is the imaginary unit, S_{-n} is the spin lowering operator at site n, and $|0\rangle$ is the ground state. The periodic boundary condition ensures that, $e^{ipN} = 1$. This ensures that the momentum are quantized,

$$e^{ipn} = e^{ip(n+N)}$$

which implies that the momentum p is quantized in units of $\frac{2\pi}{N}$. Thus, the allowed values for p are:

$$p = \frac{2\pi k}{N}, \quad k = 0, 1, 2, \ldots, N-1$$

The energy corresponding to each allowed value of p is given by the dispersion relation:

$$E(p) = 2J \sin^2\left(\frac{p}{2}\right)$$

Substituting the quantized values of p, we get the energy levels for the magnon as:

$$E_k = 2J \sin^2\left(\frac{\pi k}{N}\right), \quad k = 0, 1, 2, \ldots, N-1$$

For $N = 3$ case, in the basis of magnon, write the Markov chain associated with transitions between magnons. You can assume Boltzmann type transition between magnons, where the elements of P have the form:

$$P_{ij} \sim e^{-(E_k - E_{k'})/k_B T}.$$

Remember, in the ring configuration, the energy is at maximum at $k = N/2$ because this is the case where exactly half of the spins are flip. What are the difference between transition matrices in site basis and in magnon basis?

Question 5: Markov chain in magnon basis

Again, at a given temperature, find a stationary distribution π by solving the following expression,

$$\pi P = \pi, \quad \text{and} \quad \sum_{i=1}^{k} \pi_i = 1.$$

How does the stationary distribution of magnon changes as you increase the temperature? What are the similarities and difference from the site basis above? Remember, you are in the magnon basis.

Question 6: Markov chain in magnon basis

Use the power iteration,

$$\pi_{k+1} = \pi_k P$$

, to find the stationary distribution for the following three initial guesses,

- 1) $\Pr(|k=1\rangle) = 1$,
- 2) $\Pr(|k=1\rangle) = \frac{1}{2}, \Pr(|k=4\rangle) = \frac{1}{2}$,
- 3) a uniformly distributed initial magnon configuration.

Question 7: Master equation evolution

The classical master equation in continuous time takes the general form,

$$\frac{d\pi_i}{dt} = \sum_j \left(Q_{ji}\pi_j - Q_{ji}\pi_i\right).$$

Convert the previous transition matrix P into the transition rate matrix Q numerically. Be careful on the "time" definition when you use P^n. Hint: try to fix n, and find the relation with respect to $t \sim n\Delta t$,

$$Q \sim \frac{1}{n\Delta t} \ln(P^n). \tag{5}$$

Write the linear equation in the following matrix representation,

$$\frac{d\pi}{dt} = \pi Q, \tag{6}$$

and with the initial condition $\Pr(|k=1\rangle) = 1$, solve the above system numerically with any **scipy** integrator, and visualize the probability π_i.