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Exercise class in HCI J7.

Exercise 1. ***Continuous time Quantum Monte Carlo***

We will solve the 0D quantum Hamiltonian

$$H = -\frac{h}{2}\sigma_z - \frac{\Gamma}{2}\sigma_x \tag{1}$$

by mapping it to a classical 1D Ising model and using a continuous-time segment update Monte Carlo method, as discussed in the lecture.

1. Map the single quantum spin Hamiltonian H to the 1D Ising chain of length M at inverse temperature β_{cl} with Hamiltonian

$$H_{cl} = -J_{cl}\sum_{i=1}^{M}\sigma_i\sigma_{i+1} - h_{cl}\sum_{i=1}^{M}\sigma_i + E_0 \tag{2}$$

i.e. derive equations (7.27)-(7.29) from the script.

2. Using the map to the 1D problem, verify that the energy difference when adding or removing a pair of domain walls, $n \to n+2$ or $n \to n-2$, is given by

$$\Delta E = -\frac{h}{2}\Delta S_z^{\text{tot}} \mp \frac{2}{\beta}\log\left(\frac{d\tau\Gamma}{2}\right), \tag{3}$$

where $S_z^{\text{tot}} = \frac{1}{\beta}\int_0^\beta d\tau\sigma(\tau)$ is the total magnetization of the 1D classical Ising model.

Hint: For a given configuration C of 1D classical spins with $2n$ domain walls, calculate the energy using H_{cl} in the limit $M \to \infty, \Delta\tau \to 0$. Then use $\beta_{cl}H_{cl} = \beta H$ to find the corresponding energy of the quantum spin. Alternatively, you can use the expression for the weight $W(C)$ from the script and the fact that $W(C) = \exp(-\beta E[C])$.

3. Implement the correct Monte Carlo update by proposing a new configuration, with domain walls either added or removed at continuous imaginary times $\tau \in [0, \beta]$. The configuration is then accepted with probability

$$A(X \to Y) = \min\left(1, \frac{V_Y T(Y \to X)}{V_X T(X \to Y)}\right) \tag{4}$$

where $V_Y/V_X = e^{-\beta\Delta E}$ and $X = 2n, Y = 2n+2$ or $2n-2$, with $2n$ describing the even number of domain walls. In the case of a new configuration with two additional domain walls, $2n \to 2n+2$, the transition probability is given by the probability of picking two imaginary time locations

τ_1, τ_2, $T(X \to Y) = (d\tau/\beta)^2$. The reverse process with $T(Y \to X) = 1/((2n+1)(2n+2))$ describes the transition probability of removing two domain walls, selected subsequently out of the $2n+2$ available transitions. The case of a configuration with two removed domain walls $2n \to 2n-2$ can be found accordingly.

4. After a suitable thermalization, use the generated samples to measure the magnetization $\langle \sigma_x \rangle$. You should be able to reproduce the exact solution

$$\langle \sigma_x \rangle = \frac{\Gamma}{\sqrt{\Gamma^2 + h^2}} \tanh\left(\frac{\beta}{2}\sqrt{h^2 + \Gamma^2}\right) \tag{5}$$

as a function of Γ. You can calculate the magnetization in the Monte Carlo scheme as

$$\langle \sigma_x \rangle = \frac{\langle \# \text{ of domain walls } \rangle}{\frac{\Gamma\beta}{2}} \tag{6}$$

Since Monte Carlo is a stochastic method, you should add error bars to the calculated values. To achieve this, use the binning method introduced in last week's exercise.

Reasonable values for the simulation:

- $\beta = 1$
- h = 1
- $\Gamma \in [0.05, 6]$ for 100 values