This problem set will cover more concepts regarding Gibbs states, specifically Lieb-Robinson bounds and Lindbladians. The former is closely related to the low-temperature learning algorithm from class, and the latter is supplementary material meant to expose you to the adjacent area of *Gibbs sampling* which is closely related to some of the ideas from the low-temperature material.

The questions have been labeled with the date of the lecture in which the relevant material is covered, to help you budget your time. The questions are meant to be challenging, so do not feel discouraged if you get stuck and are unable to solve some of them.

If you find that you are running low on time to finish all the problems, our recommendation is to try to aim for breadth rather than depth – e.g., it is better to complete a few parts of each of the three questions, than to completely solve one of the three questions and skip the others.

Below we provide hints for the various problems in this assignment. While these may help you solve the problems more easily, you are not required to follow the hints as long as the proofs you provide are correct.

1 (40 PTS.) LIEB-ROBINSON BOUNDS (10/29)

Notation. Consider Hamiltonian $H = \sum_a \lambda_a P_a$ with coefficients satisfying $|\lambda_a| \leqslant 1$. Recall that the *dual interaction graph* of H is the graph whose vertices correspond to the terms $\{P_a\}$, and whose edges connect terms P_a and P_b that have overlapping support. The *interaction degree* $\mathfrak{d}$ of H is the degree of this graph. We say that two vertices in the graph have distance ℓ if the shortest path between them is of length ℓ. We say that a vertex has distance ℓ from a *subset S of qubits* if the minimum of its distances to all of the terms P_a which overlap with S is ℓ.

Recall the statement of the Lieb-Robinson bound from class.

Lemma 1.1 (Lieb-Robinson bound). *Let $t \in \mathbb{R}$. For any operator A acting on subsystem $S \subseteq [n]$ and satisfying $\|A\|_{\mathsf{op}} \leqslant 1$, if H_ℓ is given by removing all terms from H at distance at least ℓ from S, then*

$$\|A_{H_\ell}(t) - A_H(t)\|_{\mathsf{op}} \leqslant |S| \cdot \frac{O(\mathfrak{d}|t|)^\ell}{\ell!}.$$

The goal of this exercise will be to prove a weak version of the result for short times t and very local operators A. We will also explore consequences for bounds on *imaginary* time-evolved operators.

Below, let A be an operator that only acts on a single qubit, that is, $|S| = 1$. Suppose as before that $\|A\|_{\mathsf{op}} \leqslant 1$.

1.A. (5 PTS.) **Time derivative of time evolution.** Verify the identity

$$\frac{\partial}{\partial t} A_H(t) = i[H, A_H(t)]$$

One can thus deduce from Taylor's theorem that

$$A_H(t) = A + \sum_{k=1}^{\infty} \frac{(it)^k}{k!} \underbrace{[H, [H, \cdots [H,}_{k \text{ times}} A] \cdots] := A + \sum_{k=1}^{\infty} \frac{(it)^k}{k!} [H, A]_k.$$

1.B. (12 PTS.) **Lower-order terms agree.** Prove that for $k < \ell$, $[H, A]_k = [H, A]_\ell$.

1.C. (15 PTS.) **Controlling higher-order terms.** Prove that for $\ell \geqslant \ell$, $\|[H, A]_k\|_{\mathsf{op}}, \|[H_\ell, A]_k\|_{\mathsf{op}} \leqslant \ell! \cdot O(\mathfrak{d})^\ell$.

1.D. (3 PTS.) **Finishing the proof for small times.** Deduce that there is some absolute constant $c > 0$ such that for any t, possibly complex-valued, for which $|t| \leqslant c/\mathfrak{d}$,

$$\|A_{H_\ell}(t) - A_H(t)\|_{\mathsf{op}} \leqslant O(\mathfrak{d}|t|)^\ell.$$

1.E. (5 PTS.) **Bound on imaginary time evolution** Using Part 1.C., deduce that for $\rho = e^{-\beta H}/\operatorname{tr} e^{-\beta H}$,

$$\|\rho A \rho^{-1}\|_{\mathsf{op}} \leqslant \frac{1}{1 - C\mathfrak{d}\beta}$$

for some absolute constant $C > 0$.

Solution:

   1.A.

   1.B.

   1.C.

   1.D.

   1.E.

2 (40 PTS.) LOCAL LINDBLADIANS FOR SPIN CHAINS: DEPHASING, DETAILED BALANCE, AND MIXING (10/29)

Motivation: Open quantum spin chains provide a clean setting to see how Hamiltonian dynamics, noise, and thermalization interact. In this problem you will (i) diagonalize a translation-invariant dephasing Lindbladian on a 1D spin chain, (ii) see why adding only dephasing to a commuting Hamiltonian can lead to many steady states, and (iii) build a nearest-neighbor Gibbs sampler (a Davies–type generator) whose unique fixed point is (morally) the Gibbs state of an Ising chain. You will then relate the spectral gap of the full Lindbladian to the classical Glauber gap and a dephasing rate, and finish with a single-qubit example providing a concrete instantiation of these bounds.

Setup: Let $\Lambda = \{1, \ldots, n\}$ be a ring of n qubits with periodic boundary conditions. Denote Pauli operators by X_i, Y_i, Z_i acting on site i. A *Lindbladian* is a matrix-valued function of the form

$$\mathcal{L}(\rho) = -i[H, \rho] + \sum_\ell \gamma_\ell \left(L_\ell \rho L_\ell^\dagger - \tfrac{1}{2}\{L_\ell^\dagger L_\ell, \rho\} \right),$$

where the L_ℓ's are called *jump operators*; this defines an evolution of density matrices given by

$$\frac{d\rho(t)}{dt} = \mathcal{L}(\rho(t)).$$

Throughout, we let H be the Ising Hamiltonian

$$H_{\text{Ising}} = -J \sum_{i \in \Lambda} Z_i Z_{i+1} - h \sum_{i \in \Lambda} Z_i,$$

with indices defined modulo n, and the *uniform on-site dephasing* Lindbladian with jump operators $L_i^{\text{deph}} = Z_i$ at rate $\gamma > 0$:

$$\mathcal{D}_{\text{deph}}(\rho) = \gamma \sum_{i \in \Lambda} \left(Z_i \rho Z_i - \rho \right).$$

For any Pauli string $P = \bigotimes_{i=1}^n \sigma_i$ with $\sigma_i \in \{I, X, Y, Z\}$, let

$$k_{XY}(P) := \left| \{i : \sigma_i \in \{X, Y\}\} \right|$$

which we call the *coherence order* of P. We will also use single-spin flip operators $\sigma_i^\pm = \frac{1}{2}(X_i \pm iY_i)$ and the local neighbor projectors

$$P_{i-1,i+1}^{(\uparrow\uparrow)} = \tfrac{1}{4}(I + Z_{i-1})(I + Z_{i+1}), \quad P_{i-1,i+1}^{(\uparrow\downarrow)} = \tfrac{1}{4}(I + Z_{i-1})(I - Z_{i+1}), \quad \text{etc.}$$

There are four such projectors; together they resolve the identity on sites $i \pm 1$.

Primer. *Stationary state for a Lindbladian:* $\rho_\star$ is stationary if $\mathcal{L}(\rho_\star) = 0$.
Classical continuous-time Markov chain: On a finite state space Ω, a generator $Q = (Q_{x,y})_{x,y \in \Omega}$ has $Q_{x,y} \geqslant 0$ for $x \neq y$ and rows summing to zero: $Q_{x,x} = -\sum_{y \neq x} Q_{x,y}$. Probabilities evolve by the master equation $\dot{p}_t = p_t Q$. A distribution π is *stationary* if $\pi Q = 0$. *Detailed balance* with respect to π means $\pi_x Q_{x,y} = \pi_y Q_{y,x}$; this implies $\pi Q = 0$. The *spectral gap* of Q is the smallest nonzero value of $-\operatorname{Re}\lambda$ over $\lambda \in \operatorname{spec}(Q)$; it governs exponential mixing to π.

2.A. (8 PTS.) **Warm-up: spectrum of translation-invariant dephasing.** Consider $\mathcal{L}_0 := \mathcal{D}_{\text{deph}}$ with $H = 0$.

(i) Show that every Pauli string P is an eigenoperator of $\mathcal{L}_0$ and compute its eigenvalue

$$\mathcal{L}_0(P) = -2\gamma\, k_{XY}(P)\, P.$$

Here $k_{XY}(P)$ is the number of sites where P contains X or Y. Letting $\rho(0) = \sum_P c_P(0) P$, solve $\frac{d\rho(t)}{dt} = \mathcal{L}_0(\rho(t))$ for the $c_P(t)$'s and comment on their decay properties.

(ii) Compute the multiplicity of the eigenvalue $-2\gamma k$ of $\mathcal{L}_0$.
Hint: count Pauli strings with exactly k letters in $\{X, Y\}$.

2.B. (8 PTS.) **Commuting Hamiltonians + dephasing: many steady states.** Let $\mathcal{L}_{\text{comm}} := -i[H_{\text{Ising}}, \cdot] + \mathcal{D}_{\text{deph}}$.

(i) Show that the subspace $\operatorname{Diag}_Z := \{\rho : \rho \text{ is diagonal in the common eigenbasis of all } Z_i\}$ is invariant under $\mathcal{L}_{\text{comm}}$, and that $\mathcal{L}_{\text{comm}}$ acts as zero on Diag_Z.

(ii) Conclude that *every* classical probability distribution over spin configurations (embedded as a diagonal density matrix in the Z basis) is a stationary state, and compute the dimension of the fixed point space (as a vector space; and as physical states with trace one).

(iii) Argue that all non-diagonal Pauli strings decay at least at rate 2γ, i.e. the nonzero part of the spectrum of $\mathcal{L}_{\text{comm}}$ lies in $\{\lambda : \operatorname{Re}\lambda \leqslant -2\gamma\}$.

2.C. (10 PTS.) **A local Gibbs sampler for the Ising chain.** We now add local, neighbor-conditioned spin-flip jumps. For each site i and each neighbor configuration $s \in \{\uparrow\uparrow, \uparrow\downarrow, \downarrow\uparrow, \downarrow\downarrow\}$, set

$$L_{i,s}^{\uparrow} = \sqrt{r_s^{\uparrow}}\, P_{i-1,i+1}^{(s)}\, \sigma_i^{+}, \qquad L_{i,s}^{\downarrow} = \sqrt{r_s^{\downarrow}}\, P_{i-1,i+1}^{(s)}\, \sigma_i^{-},$$

and define

$$\mathcal{L}_\beta(\rho) := -i[H_{\mathrm{Ising}}, \rho] + \mathcal{D}_{\mathrm{deph}}(\rho) + \sum_{i,s}\left(L_{i,s}^{\uparrow}\, \rho\, L_{i,s}^{\uparrow\dagger} - \tfrac{1}{2}\{L_{i,s}^{\uparrow\dagger} L_{i,s}^{\uparrow}, \rho\}\right) + \sum_{i,s}\left(L_{i,s}^{\downarrow}\, \rho\, L_{i,s}^{\downarrow\dagger} - \tfrac{1}{2}\{L_{i,s}^{\downarrow\dagger} L_{i,s}^{\downarrow}, \rho\}\right).$$

Let $S(s) \in \{-2, 0, +2\}$ denote the sum of neighbor spins in configuration s (eigenvalues ± 1 of Z). Flipping i from $\downarrow$ to $\uparrow$ when neighbors are s changes the evaluation of the Hamiltonian by

$$H_{\mathrm{Ising}}(\uparrow; s) - H_{\mathrm{Ising}}(\downarrow; s) = -2\big(h + J S(s)\big).$$

We fix explicit "heat-bath" rates

$$r_s^{\uparrow} = \kappa\, \frac{e^{\beta(h + JS(s))}}{2\cosh\big(\beta(h + JS(s))\big)}, \qquad r_s^{\downarrow} = \kappa\, \frac{e^{-\beta(h + JS(s))}}{2\cosh\big(\beta(h + JS(s))\big)}, \tag{1}$$

for some $\kappa > 0$ (overall time scale). We see that the rates (1) obey the local detailed balance condition

$$\frac{r_s^{\uparrow}}{r_s^{\downarrow}} = e^{-\beta\,(H_{\mathrm{Ising}}(\uparrow;s) - H_{\mathrm{Ising}}(\downarrow;s))} = e^{2\beta\,(h + J\,S(s))}.$$

(i) **Restriction to diagonal probabilities.** Let $\rho_t = \sum_{z \in \{\uparrow,\downarrow\}^n} p_t(z)\, |z\rangle\langle z|$ be diagonal. Show directly from the definition of $\mathcal{L}_\beta$ that the diagonal entries evolve as

$$\frac{d}{dt} p_t(z) = \sum_{i=1}^{n}\left(p_t(z^{(i\downarrow)})\, r_{s_i(z^{(i\downarrow)})}^{\uparrow} + p_t(z^{(i\uparrow)})\, r_{s_i(z^{(i\uparrow)})}^{\downarrow} - p_t(z)\left(r_{s_i(z)}^{\uparrow}\, \mathbf{1}_{z_i=\downarrow} + r_{s_i(z)}^{\downarrow}\, \mathbf{1}_{z_i=\uparrow}\right)\right),$$

where $z^{(i\uparrow)}$ (respectively $z^{(i\downarrow)}$) is z with spin i set to $\uparrow$ (respectively $\downarrow$), and $s_i(\cdot)$ reads the neighbors of i. Conclude that the restriction of $\mathcal{L}_\beta$ to Diag_Z is a classical continuous-time Markov chain with generator Q whose nonzero off-diagonal entries flip a single spin with the rates in (1).

(ii) **Stationarity of the Gibbs distribution.** Let $\pi_\beta(z) \propto e^{-\beta H_{\mathrm{Ising}}(z)}$. Using (i) and the definition of Q, show that for configurations x, y that differ by one spin flip,

$$\pi_\beta(x)\, Q_{x,y} = \pi_\beta(y)\, Q_{y,x}.$$

This detailed balance identity implies $\pi_\beta Q = 0$. Conclude that the Gibbs state $\rho_\beta = \frac{e^{-\beta H_{\mathrm{Ising}}}}{\mathrm{tr}(e^{-\beta H_{\mathrm{Ising}}})}$ is stationary for $\mathcal{L}_\beta$, namely $\mathcal{L}_\beta(\rho_\beta) = 0$.

2.D. (8 PTS.) **Decomposition and the mixing/spectral gap.** Let $\mathrm{gap}(\mathcal{M})$ denote the spectral gap of a generator $\mathcal{M}$, i.e., the smallest nonzero value of $-\mathrm{Re}\,\lambda$ over $\lambda \in \mathrm{spec}(\mathcal{M})$.

(i) Show that Diag_Z and its Hilbert–Schmidt orthogonal complement Off_Z are invariant subspaces of $\mathcal{L}_\beta$.

(ii) Prove that the spectrum of $\mathcal{L}_\beta$ contains the spectrum of the classical generator Q (acting on Diag_Z).

(iii) Show that all eigenvalues of $\mathcal{L}_\beta$ on Off_Z satisfy $\mathrm{Re}\,\lambda \leqslant -2\gamma$. *Hint:* The Hamiltonian commutator is anti-Hermitian (purely imaginary); dephasing contributes $\leqslant -2\gamma$ to real parts; the extra dissipators are contractive.

(iv) Conclude that $\mathrm{gap}(\mathcal{L}_\beta) = \min\{\, 2\gamma,\ \mathrm{gap}(Q)\, \}$.

2.E. (6 PTS.) **Single-site check: Heisenberg equation for Z.** Consider a single qubit with $H = 0$ and jump operators $L^{\uparrow} = \sqrt{\gamma_\uparrow}\,\sigma^{+}$, $L^{\downarrow} = \sqrt{\gamma_\downarrow}\,\sigma^{-}$. Work in the Heisenberg picture, where the dual generator acts as

$$\mathcal{L}^*(O) = \sum_{\alpha \in \{\uparrow,\downarrow\}} \gamma_\alpha\left(L^{\alpha\dagger} O L^\alpha - \tfrac{1}{2}\{L^{\alpha\dagger} L^\alpha, O\}\right).$$

Show that

$$\mathcal{L}^*(Z) = -(\gamma_\uparrow + \gamma_\downarrow)\, Z + (\gamma_\uparrow - \gamma_\downarrow)\, I,$$

and deduce the ODE

$$\frac{d}{dt}\langle Z\rangle_t = -(\gamma_\uparrow + \gamma_\downarrow)\langle Z\rangle_t + (\gamma_\uparrow - \gamma_\downarrow)$$

with fixed point $\langle Z\rangle_\infty = \frac{\gamma_\uparrow - \gamma_\downarrow}{\gamma_\uparrow + \gamma_\downarrow}$. (If you choose $\gamma_\uparrow/\gamma_\downarrow = e^{2\beta h}$, verify that $\langle Z\rangle_\infty = \tanh(\beta h)$, consistent with a one-site Gibbs state.)

Solution:

2.A.

2.B.

2.C.

2.D.

2.E.