## Problem 1. High temperature Schrödinger dynamics.

This problem considers general properties of the dynamics of thermal density matrices.

(a) Show that all observables initially in a thermal equilibrium quantum state of an (arbitrary) Hamiltonian $H$ are static in time when evolved under $H$.

(b) Consider a state $\rho_0$ initially in thermal equilibrium for a Hamiltonian $H_0$ at time $t = 0$. Starting at time $t = 0$ let the state evolve under a potentially different Hamiltonian $H_1$. Show that if the initial temperature is infinite, all observables are time-independent.

(c) Under the same scenario as the previous part, but at finite initial state temperature $T$, solve for the dynamics of $\langle O(t)\rangle$ in terms of $H_0$, $H_1$, $T$, and $t$. (A formal solution in terms of these quantities is fine since we haven't specified any of their values, or even the Hilbert space.)

## Problem 2. Density matrix properties.

In class, we derived density matrices to describe two situations: (i) a pure quantum state $c$ randomly given with some probability $p_c$, and (ii) in large quantum systems (both pure and mixed ones) consisting of a "system" and "bath," where we want to consider observables acting only on the "system."

In the first case, the density matrix was given by

$$\rho_{\text{stoch}} = \sum_c p_c \left|c\right\rangle \left\langle c\right| , \tag{1}$$

while in the second it is

$$\rho_S = \text{Tr}_E \rho \tag{2}$$

where $\rho$ is the density of the full system-environment universe, and $\text{Tr}_E$ indicates tracing over the environment degrees of freedom.

Here, you will derive some of the basic properties of these density matrices.

(a) Show that both density matrices ($\rho_{\text{stoch}}$ and $\rho_S$) have the following properties:

- $\rho = \rho^\dagger$
- $\text{Tr}[\rho] = 1$
- $\rho$ is a positive operator, i.e. $\langle\psi|\rho|\psi\rangle \geq 0$ for all $\psi$.
- $\langle a|\rho^2|b\rangle \leq \langle a|\rho|b\rangle$
- The matrix elements satisfy: $|\rho_{ab}|^2 \leq \rho_{aa}\rho_{bb}$ with equality only when the density matrix describes a pure state.

  *Hint: if you get stuck on inequalities, Cauchy-Schwarz them!*

  We refer to the diagonal matrix elements $\rho_{aa}$ as occupancies (of state $a$), while we refer to the off-diagonal matrix elements $\rho_{ab}$ as coherences (between states $a$ and $b$). Thus pure states maximize coherence.

It is actually possible to present quantum mechanics *starting* with density matrices as the *states* of the quantum system, replacing vectors in the Hilbert space as the "states" of the theory. One defines these states (density matrices) as satisfying a set of axioms; these axioms are a subset of those that you checked above (the first three suffice – see Nielsen and Chuang). Such a formalism is fairly natural, considering how ubiquitous open systems are, although I am not aware of a book that proceeds this way.

(b) In the Schrödinger picture, states evolve while observables are static. Thus, the density matrix evolves (it is associated with the state). Derive the time evolution differential equation for the density matrix (sometimes called the von Neumann equation). Discuss similarities and differences of the density matrix in the Schrödinger picture with the evolution of observables in the Heisenberg picture.

(c) How does the density matrix transform under a symmetry transformation? *Hint: recall how symmetries act on pure states, and consider unitary and anti-unitary symmetries case-by-case.*

## Problem 3. Bloch vector dynamics.

In this problem, we will derive the dynamics of the Bloch vector (which has simple geometric and physical interpretations) from the Schrödinger equation.

Consider a spin-1/2 in a magnetic field $\vec{H}$. The Hamiltonian is

$$H = \gamma \vec{H} \cdot \vec{S} \tag{3}$$

where $\vec{S} = (1/2)\vec{\sigma}$ with $\vec{\sigma} = \{\sigma^x, \sigma^y, \sigma^z\}$ are the Pauli matrices. This is the Hamiltonian of a spin with gyromagnetic ratio $\gamma$.

In lecture we will show that the density matrix can be uniquely represented as a "Bloch vector" $\vec{\mathcal{B}}$, with a precise mathematical definition through

$$\rho = \frac{1}{2}\left(\mathbb{1} + \vec{\mathcal{B}} \cdot \vec{\sigma}\right) \tag{4}$$

where $\mathbb{1}$ is the identity matrix.

(a) Using this definition of the Bloch vector, show that the Schrödinger equation gives equations of motion for the Bloch vector

$$\partial_t \vec{\mathcal{B}} = \frac{\gamma}{2} \vec{H} \times \vec{\mathcal{B}}. \tag{5}$$

And please check my factors of two!

(b) Pictorially describe the solutions of these equations for an arbitrary initial Bloch vector.

(c) (Qualitatively) guess how one might add damping/dissipation of any kind to these equations.

Actually, this equation can be derived using only operator properties (commutators) without ever specifying a Hilbert space. Thus it is equally true for higher spins (spin-1, spin-3/2, ...), as long as the Hamiltonian remains Eq. (4). The only difference is that while for spin-1/2 Eq. (4) is the most general Hamiltonian, for higher spins, other terms can be added, e.g. $(S^z)^2$. (For a spin-1/2, $(S^z)^2 = 1$.)

## Problem 4. Effect of noise (and warmup for spectroscopy)

Consider a spin-1/2. Initially put it in the state $|{\rightarrow}\rangle = (1/\sqrt{2})(|{\uparrow}\rangle + |{\downarrow}\rangle)$.

(a) Let the spin evolve under the Hamiltonian

$$H = \begin{pmatrix} 0 & 0 \\ 0 & \Delta \end{pmatrix} \tag{6}$$

for a time $t$. Calculate $\langle S^x(t)\rangle$, $\langle S^y(t)\rangle$, and $\langle S^z(t)\rangle$. (You may solve directly or use your results from above.)

(b) Now imagine that you do this measurement many times. Each time you do the experiment, you have a different value of $\Delta$, although $\Delta$ is constant in time for each experiment. The $\Delta$ in each experiment is sampled from the probability distribution

$$P(\Delta) = \frac{1}{\sqrt{2\pi}\sigma_\Delta} e^{-\Delta^2/(2\sigma_\Delta^2)}. \tag{7}$$

What are $\langle S^x(t)\rangle$, $\langle S^y(t)\rangle$, and $\langle S^z(t)\rangle$ averaged over many runs of your experiment?

Note that the noise of the shot-to-shot fluctuating $\Delta$ causes damping. This is our first taste of an open quantum system. In many cases, not only will $\Delta$ vary shot-to-shot, but will vary randomly with time in a given experiment. One can in principle treat this problem by breaking the time evolution into $N$ slices of duration $t/N$, then taking the large-$N$ limit. Indeed stochastic calculus techniques (Wiener processes, Ito/Strotonavitch, etc.) arise as essentially the formalism to take this limit. This is very similar to what we usually do in calculus, except the "continuum limit" for this stochastic case is less familiar (the curves that result from such random processes are everywhere non-differentiable, and limits don't work in the usual way.) We will deal with such noisy dynamics later in this course and connect it to the evolution of a quantum system coupled to a large environment or reservoir.