Statistical Mechanics - 2019-2 - Problem set 2

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Deadline: 15/10

1. **Quantum master equation:** In class we discussed master equations in the context of the evolution of probabilities p_n. However, these master equations can also be cast in terms of an evolution of the full density matrix $\rho(t)$. This is called a Quantum (or Lindblad) Master equation. Here we shall study as an example the harmonic oscillator. Its master equation reads

$$\frac{d\rho}{dt} = \mathcal{L}(\rho) = \gamma(\bar{N}+1)\Big[a\rho a^\dagger - \frac{1}{2}\{a^\dagger a, \rho\}\Big] + \gamma\bar{N}\Big[a^\dagger\rho a - \frac{1}{2}\{aa^\dagger, \rho\}\Big], \tag{1}$$

where $\{A, B\} = AB + BA$ is the anti-commutator, $\bar{N} = (e^{\beta\hbar\omega} - 1)^{-1}$ is the Bose-Einstein distribution and $\gamma > 0$ is a constant measuring the coupling strength to the reservoir[1].

   (a) Check that this equation preserves the trace. That is, if $\text{tr}(\rho(0)) = 1$, then for all future times $\text{tr}(\rho(t)) = 1$. In addition to this, in order for Eq. (1) to represent a valid evolution equation for any density matrix, it must also preserve positivity. That is, if $\rho(0) \geq 0$ then $\rho(t) \geq 0$ for any t. This turns out to be true for (1) as well, although the proof is slightly more difficult.

   (b) Using $[a, a^\dagger] = 1$ show that

$$e^{\beta\hbar\omega a^\dagger a} a e^{-\beta\hbar\omega a^\dagger a} = e^{-\beta\hbar\omega} a. \tag{2}$$

   (c) Use the previous result to show that $\rho \propto e^{-\beta\hbar\omega a^\dagger a}$ is a fixed point of Eq. (1). That is $\mathcal{L}(e^{-\beta\hbar\omega a^\dagger a}) = 0$. Moreover, show that this is true if and only if the β in $e^{-\beta\hbar\omega a^\dagger a}$ is the same as the one in $\bar{N}$.

   (d) Consider now the populations $p_n(t) = \langle n|\rho(t)|n\rangle$. Show that the populations evolve according to the same master equation we studied in class. Namely,

$$\frac{dp_n}{dt} = \gamma(\bar{N}+1)\Big\{(n+1)p_{n+1} - np_n\Big\} + \gamma\bar{N}\Big\{np_{n-1} - (n+1)p_n\Big\}. \tag{3}$$

   (e) Next consider average occupation $\langle a^\dagger a\rangle = \text{tr}\{a^\dagger a\rho\}$. Show from either Eq. (1) or Eq. (3) that it evolves according to

$$\frac{d\langle a^\dagger a\rangle}{dt} = \gamma(\bar{N} - \langle a^\dagger a\rangle). \tag{4}$$

   Solve it and discuss the result.

2. **Spontaneous emission:** When atoms are coupled to the electromagnetic field, they may emit or absorb a photon. The quantum master equation describing this process, assuming a two-level atom, is very similar to Eq. (1):

$$\frac{d\rho}{dt} = \gamma(\bar{N}+1)\Big[\sigma\rho\sigma^\dagger - \frac{1}{2}\{\sigma^\dagger\sigma, \rho\}\Big] + \gamma\bar{N}\Big[\sigma^\dagger\rho\sigma - \frac{1}{2}\{\sigma\sigma^\dagger, \rho\}\Big], \tag{5}$$

but now $\sigma = |0\rangle\langle 1|$ is the lowering operator for a 2-level atom and, as before, $\bar{N} = (e^{\beta\epsilon} - 1)^{-1}$. The terms proportional to $\bar{N}$ are called stimulated emission and absorption, whereas the factor of "1" in $\bar{N}+1$ is the **spontaneous emission**. This term is related to the coupling of the atom to the electromagnetic vacuum and therefore persists even at zero temperature.

   (a) The excited state population is described by the operator $\sigma^\dagger\sigma = |1\rangle\langle 1|$. Show that the evolution of $\langle\sigma^\dagger\sigma\rangle$ is described by the equation

$$\frac{d\langle\sigma^\dagger\sigma\rangle}{dt} = \gamma(2\bar{N}+1)\Big[\frac{\bar{N}}{2\bar{N}+1} - \langle\sigma^\dagger\sigma\rangle\Big]. \tag{6}$$

   What is the steady-state of Eq. (6)? Does it make sense?

[1] In principle there can also be a Hamiltonian term in Eq. (1) describing the unitary evolution. I omit it because I don't want you to worry about that. The final results in this case will also be independent of it, so it's not a problem to neglect it.

(b) Solve Eq. (6) and show that the effective relaxation rate depends on temperature. Analyze the limit $\bar{N} = 0$.

(c) The density matrix for a qubit can always be written as

$$\rho = \begin{pmatrix} 1-p & q \\ q^* & p \end{pmatrix}, \tag{7}$$

where $p = \langle \sigma^\dagger \sigma \rangle$ is the population of the excited state and $q = \langle \sigma^\dagger \rangle$ is the coherence in the population basis. Study the evolution of q under the master equation (5). You will find that q decays exponentially. This process is called **decoherence**. When a system is coupled to a bath, in addition to the populations adjusting to those imposed by the bath, the quantum coherences are also destroyed.

(d) Now parametrize the density matrix as

$$\rho = \frac{1}{2}\begin{pmatrix} 1+s_z & s_x - i s_y \\ s_x + i s_y & 1 - s_z \end{pmatrix}, \tag{8}$$

where, as we saw in class, $s_i = \langle \sigma_i \rangle$ are the expectation values of the Pauli matrices. Use your results from (b) and (c) to discuss how is the trajectory of the qubit in Bloch's sphere.

3. **Entropy production and decoherence:**[2] In class we saw how to model the entropy production during the relaxation dynamics. But in that case we were considering only classical master equations (i.e., the dynamics of the populations p_n). One can formulate the problem equally when in terms of quantum master equations and the evolution of the density matrix. In this case the entropy production rate becomes

$$\Pi = -\frac{d}{dt} S(\rho || \rho_{\rm th}), \tag{9}$$

where $S(\rho||\rho_{\rm th}) = {\rm tr}(\rho \ln \rho - \rho \ln \rho_{\rm th})$ is the quantum relative entropy. Consider the spontaneous emission master equation (5) and the solutions you found on exercises 2(a) and 2(c). *Show that decoherence always increases the entropy production.* Irreversibility at the quantum level therefore has an extra component related to the loss of quantum features. If you want to learn more about this, check out this paper.

4. **Superradiance:** The evolution of a the population of a single atom, at zero temperature, was found in Eq. (6). With $\bar{N} = 0$ it reads

$$\frac{{\rm d}\langle \sigma^\dagger \sigma \rangle}{{\rm d}t} = -\gamma \langle \sigma^\dagger \sigma \rangle. \tag{10}$$

Thus, the **emitted power** is proportional to $\langle \sigma^\dagger \sigma \rangle$, which is the excited state population of a single atom. As a consequence, if we now have $\mathcal{N}$ atoms in our sample, the total emitted power will be proportional to $\mathcal{N}$.

When $\mathcal{N}$ atoms are placed very close to each other however, they will have the tendency to emit to the same electromagnetic modes. The emission then becomes a collective effect. This is the idea behind superradiance: the collective emission of many atoms onto the same electromagnetic mode.

The evolution in this case can be described in terms of the so-called Dicke states $|n\rangle$, where $n = 0, 1, 2, \ldots, \mathcal{N}$ represents the *number* of atoms in the excited state. The collective dynamics will be described by the following master equation:

$$\frac{{\rm d}\rho}{{\rm d}t} = \kappa \Big[S_- \rho S_+ - \frac{1}{2}\{S_+ S_-, \rho\} \Big], \tag{11}$$

where $S_\pm$ are collective operators that act as follows:

$$S_+ |n\rangle = \sqrt{(\mathcal{N} - n)(n+1)} |n+1\rangle, \tag{12}$$

$$S_- |n\rangle = \sqrt{n(\mathcal{N} - n + 1)} |n-1\rangle. \tag{13}$$

[2] This problem is *open-ended*. This means I will not tell you exactly what *to do*, but only what *to study*. The reason why I do this is because that is how research is like. In research there is no one telling you exactly how to solve the problem; you have to figure that out by yourself.

(a) Find a differential equation for $p_n = \langle n|\rho|n\rangle$, which represents the probability of having n atoms in the excited state. You don't have to solve the equation (it is actually a bit difficult to do it).

(b) Use your result to show that the average number of atoms in the excited state, $\langle n\rangle$, evolves according to

$$\frac{\mathrm{d}\langle n\rangle}{\mathrm{d}t} = -\kappa(N+1)\langle n\rangle + \kappa\langle n^2\rangle. \tag{14}$$

As a sanity check, if $N = 1$ then $n = 0, 1$ so that $n^2 = n$. This then reduces to

$$\frac{\mathrm{d}\langle n\rangle}{\mathrm{d}t} = -2\kappa\langle n\rangle + \kappa\langle n\rangle = -\kappa\langle n\rangle,$$

which is Eq. (10).

Eq. (14) shows the main features of superradiance. First, the term proportional to $\langle n\rangle$ is amplified by a factor N. This term is the individual emission from each atom. But each atom doesn't emit with rate κ anymore, but with an effective rate $\kappa(N+1)$. The rate of emission is thus amplified by the presence of other atoms. Second, the last term in Eq. (14) is the actual superradiance. It gives a contribution to the rate $\mathrm{d}\langle n\rangle/\mathrm{d}t$ at which the atoms emit, which is proportional to $\langle n^2\rangle$. If you double the number of atoms, you quadruple the emitted power. Pretty cool eh? :)

5. **Anomalous heat flow due to quantum correlations:** Consider two qubits, with Hamiltonians $H_i = \frac{\epsilon}{2}(1-\sigma_z^i)$, where $i = A, B$.

(a) Suppose the qubits are prepared in thermal states, but at initially different temperatures T_i; that is, $\rho_i = e^{-\beta_i H_i}/Z_i$. The two qubits are then put to interact by means of a unitary $U = e^{-iHt}$, where

$$H = H_A + H_B + g(\sigma_A^+\sigma_B^- + \sigma_A^-\sigma_B^+). \tag{15}$$

Study the change in energy of A and B. Show that energy flows from the hot body to the cold body. Of course, since these are qubits, stuff will oscillate, so these conclusions have to be taken by looking at short times.

(b) Now suppose that the two qubits are initially prepared in a correlated state, of the form

$$\rho_{AB} = \rho_A^{\mathrm{th}} \otimes \rho_B^{\mathrm{th}} + \chi, \qquad \chi = \alpha|01\rangle\langle 10| + \alpha^*|10\rangle\langle 01|, \tag{16}$$

where α is a complex constant. Since $\mathrm{tr}_A\chi = \mathrm{tr}_B\chi = 0$, it follows that these states are locally thermal. Study the heat flow in this case and show that depending on the choice of α, heat may now flow from cold to hot. Notice that the values of α cannot be chosen to be too large; it must be such that ρ_{AB} is still positive semi-definite.

I think this result is super cool. Even though the two qubits are locally thermal, the fact that they are globally in a correlated state affects the flow of heat. This idea was recently tested experimentally.