

Open Quantum Systems

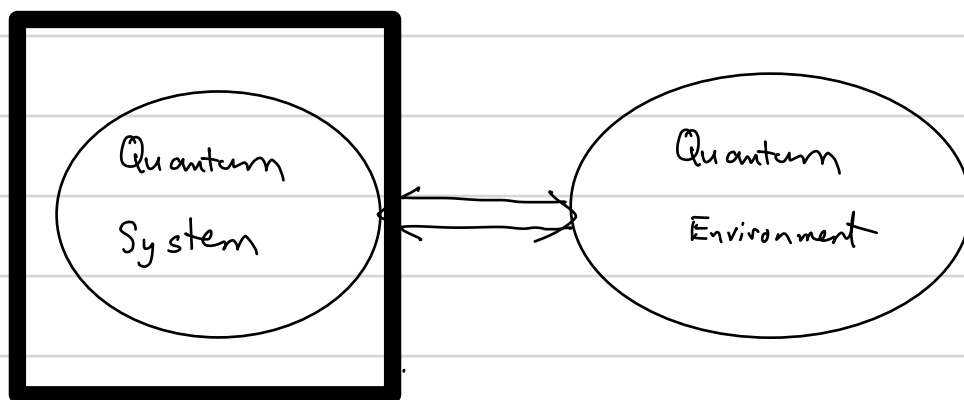
Physics 581, Spring 2023
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Lecture 1: Introduction to Open Quantum Systems

When we typically learn about quantum mechanics we learn about the Schrödinger equation. States evolve according to the dynamics generated by the Hamiltonian

$$\frac{d}{dt}|\psi\rangle = -\frac{i}{\hbar}\hat{H}|\psi\rangle \Rightarrow |\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle \quad \hat{U}(t) = e^{-\frac{i}{\hbar}\hat{H}t} \text{ (unitary)}$$

While this might be true for the whole universe, it is rarely a good approximation to the world we observe when considering quantum system. First is the tricky question of what constitutes the "system" in the first place. We divide the world in those degrees of freedom of the "system" and the rest, which we call the "environment"



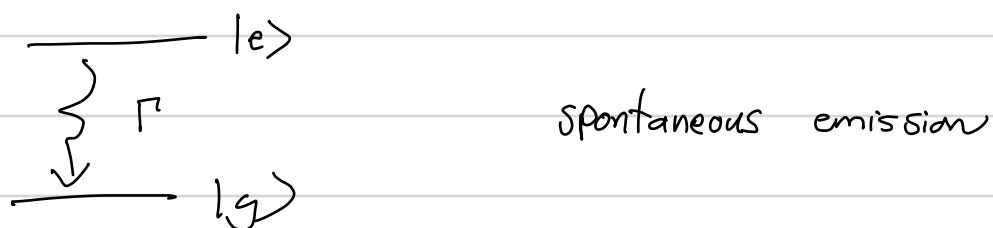
The environment may consist of the air around us, the light from the sun or radio waves from our cell phones, aqueous solutions in which molecules undergoing chemical reactions are bathed, or the phonons of a lattice that bombard a quantum dot in a solid. We may want to isolate the quantum system of interest from the environment by shielding it in a Faraday cage or magnetic μ -material, pumping out the air to create a vacuum, or using a dilution refrigerator to freeze out the unwanted degrees of freedom. But dry as we might, we can never do this perfectly, even in principle. For the vacuum is not truly the void, but teeming with quantum fluctuations. Indeed the quantum vacuum is the environment which

bathes atoms, fundamental leading to spontaneous emission.

Consider an atom in its first excited state. In the absence of any other perturbation, the excited state, let's call it $|e\rangle$, is, by definition an eigenstate of the Hamiltonian $\hat{H}|e\rangle = E_e|e\rangle$. Such states are called "stationary states" because the statistics of any measurement we would do on the atom would not change with time, because if $|\psi(0)\rangle = |e\rangle$, then according to the Schrödinger equation,

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t}|e\rangle = e^{-i\frac{E_e}{\hbar}t}|e\rangle$$

In a particular, the probability to be in the excited state $P_e(t) = |\langle e|\psi(t)\rangle|^2 = 1$ for all times. However, we know that the first excited state has a finite life-time; that is the population will decay to the ground state



In fact, in the absence of any other perturbation (e.g. collisions with background gas), the probability to be in the excited state will decay exponentially

$$P_e(t) = e^{-\Gamma t} \quad \text{where} \quad \Gamma = \frac{1}{\tau} \quad \tau = \text{Natural lifetime}$$

This decay occurs because the atom is coupled to its environment - the quantum vacuum of the electromagnetic field. It is an open quantum system. The energy in the atom is dissipated into its environment. This is one of the hallmarks of open quantum systems - Energy dissipation

Also, given initial superposition state $|\psi(0)\rangle = c_g|g\rangle + c_e|e\rangle$

$$P_e(t) = |c_e|^2 e^{-\Gamma t} \quad P_g(t) = 1 - |c_e|^2 e^{-\Gamma t} = |c_g|^2 e^{-\Gamma t} + (1 - e^{-\Gamma t})$$

Thus as $t \rightarrow \infty$ $|\psi(t)\rangle \rightarrow |g\rangle$, regardless of the initial state. Another hallmark

of open quantum systems is that their dynamics are irreversible. This is in contrast to closed quantum systems evolving according to the Schrödinger equation. Those dynamics are unitary and therefore reversible

$$|\psi(0)\rangle = \hat{U}^{-1}(t) |\psi(t)\rangle = \hat{U}^{\dagger}(t) |\psi(t)\rangle = e^{+\frac{i}{\hbar} \hat{H} t} |\psi(t)\rangle = \hat{U}(-t) |\psi(t)\rangle$$

Classical physics also shows the distinction between closed and open quantum systems. The microscopic laws of classical physics are reversible and described by Hamilton's equations of motion

$$\dot{\vec{q}} = \vec{\nabla}_p H(\vec{q}, \vec{p}), \quad \dot{\vec{p}} = -\vec{\nabla}_q H(\vec{q}, \vec{p}) \quad (\vec{q}, \vec{p}) \text{ phase space}$$

For example, the classical simple harmonic oscillator $H = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 q^2$ (one degree of freedom)

$$\dot{q} = \frac{p}{m}, \quad \dot{p} = -m\omega^2 q \Rightarrow \ddot{q} = -\omega^2 q \Rightarrow q(t) = q(0) \cos \omega t + \frac{p(0)}{m} \sin \omega t$$

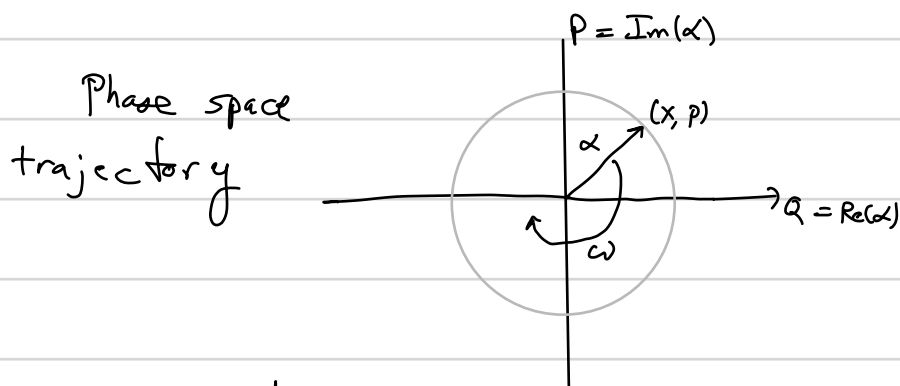
$$\ddot{p} = -\omega^2 p \Rightarrow p(t) = p(0) \cos \omega t - m\omega^2 q(0) \sin \omega t$$

If we scale units $Q = \frac{q}{q_c}, \quad P = \frac{p}{p_c} \quad m\omega^2 q_c^2 = \frac{p_c^2}{m} = E_c$

$$\dot{Q} = \omega P, \quad \dot{P} = -\omega P, \quad Q(t) = Q(0) \cos \omega t + P(0) \sin \omega t, \quad P(t) = P(0) \cos \omega t - Q(0) \sin \omega t$$

Define complex amplitude $\alpha(t) \equiv Q(t) + iP(t) = \alpha(0) e^{-i\omega t}$

Motion in phase space is the rotation of the phasor: Reversible



$$E(t) = E_c \frac{Q(t)^2 + P(t)^2}{2}$$

$$= \frac{E_c}{2} |\alpha(t)|^2 = \frac{E_c}{2} |\alpha(0)|^2$$

Energy is conserved

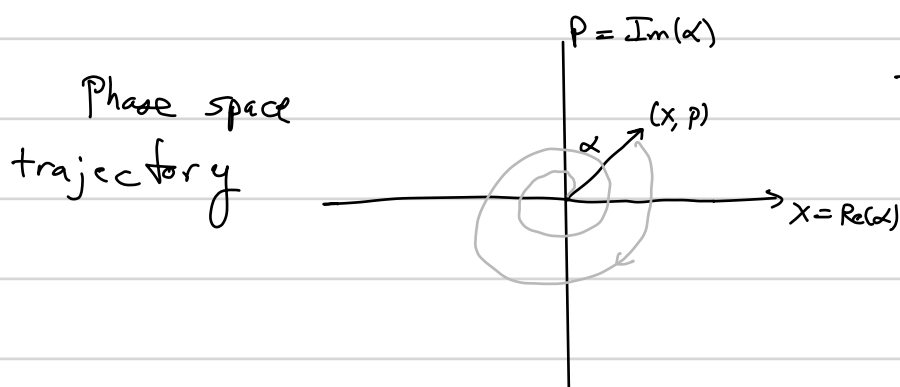
However, we know in the real world all oscillators are damped due to the viscosity of air, friction on a surface, or in a spring. The equations of motion are not Hamiltonian

$$\dot{q} = -\gamma \dot{q} + \omega^2 q, \quad \dot{p} = -\gamma \dot{p} + \omega^2 p, \quad \gamma = \text{damping rate}$$

These are equivalent to $\dot{Q} = (\omega - i\frac{\Gamma}{2})P$, $\dot{P} = -(\omega - i\frac{\Gamma}{2})Q$

or $\dot{\alpha} = -i(\omega - i\frac{\Gamma}{2})\alpha = (-i\omega - \frac{\Gamma}{2})\alpha$

$\Rightarrow \alpha(t) = \alpha(0)e^{-i\omega t - \frac{\Gamma}{2}t}$, $|\alpha(t)|^2 = |\alpha(0)|^2 e^{-\Gamma t}$



The evolution is irreversible

Energy is dissipated

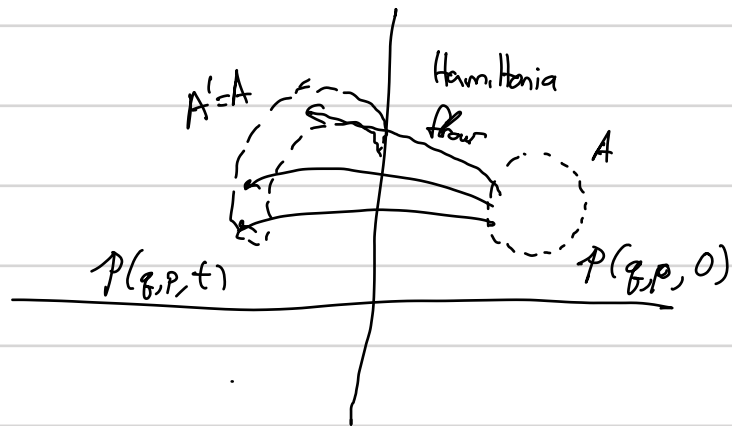
$E(t) = E(0)e^{-\Gamma t}$

In classical physics we typically include damping & dissipation phenomenologically, following from empirical laws. The fundamental microscopic laws, however are reversible, and in principle the irreversible equations of motion should be derivable, under some appropriate approximation, as an effective theory. This can be achieved through the methods of classical statistical physics, where the environment is treated as a (classically) uncertain system, but typically, the phenomenological description suffices.

Another distinction we see between open and closed system dynamics is the arrow of time. The closed system has no preferred direction of time, but in the open system time flows in one direction. The direction of time in which the amplitude decays defines the direction of time's arrow. Another place where time's arrow appears is in the second law of classical thermodynamics. Entropy increases in the forward direction of time. In a closed (reversible) Hamiltonian system, entropy is unchanged. This is reflected in Liouville's theorem which states that the area of a patch of phase space is unchanged under Hamiltonian flow. This area in phase space can be thought of as our uncertainty in the "microstate" specified by the phase space coordinates. The conservation of entropy is intimately tied to the fact that no information is lost in the

closed quantum system.

More formally, we can consider a probability distribution of phase space that evolve according to Hamiltonian flow, $\mathcal{P}(q, p, t)$



$$\text{Thus, } \mathcal{P}(q, p, t) = \mathcal{P}(q(-t), p(-t), 0)$$

$$\Rightarrow \frac{\partial}{\partial t} \mathcal{P}(q, p, t) = -\dot{q} \frac{\partial \mathcal{P}}{\partial q} - \dot{p} \frac{\partial \mathcal{P}}{\partial p} = \frac{\partial H}{\partial q} \frac{\partial \mathcal{P}}{\partial p} - \frac{\partial H}{\partial p} \frac{\partial \mathcal{P}}{\partial q} = \{H, \mathcal{P}\}_{PB}$$

$$\text{where } \{A, B\}_{PB} = \frac{\partial A}{\partial q} \frac{\partial B}{\partial p} - \frac{\partial A}{\partial p} \frac{\partial B}{\partial q} \quad \text{Poisson Bracket}$$

The equation of motion for $\mathcal{P}(q, p, t)$ is known as Liouville's eqn.

$$\text{Shannon entropy (information missing)} \quad S(t) = - \int dq dp \mathcal{P}(q, p, t) \log(\mathcal{P}(q, p, t))$$

Liouville-Hamilton equation \Rightarrow S is independent of time.

The description of open quantum systems shares much in common with the description of open classical systems, and builds on the foundation of classical statistical physics. Unifying features include

<u>Closed</u>	<u>Open</u>
Energy conserved	Energy dissipation
Time reversible	Irreversible
Entropy conserved	Entropy changes
Information conserved	Information changes

Note: In principle the entropy of the open system can increase or decrease. An example of the latter is cooling when the environment is at a lower temperature than the system.

This might be a good time to make an interlude, and discuss the second law of thermodynamics which states that for an isolated system, entropy is never decreases, and equilibrium is reached when entropy is maximized. But we just said that for a closed system (classical or quantum) entropy is unchanged and dynamics are reversible. For a closed system entropy doesn't increase, and systems never "relax" to equilibrium. This problem drove Boltzmann to madness!

So what gives? The resolution is the "thermodynamic limit." Equilibrium thermodynamics is about macroscopic systems, with a number of interacting degrees of freedom approaching infinity. (Avogadro's number will do). For such systems two things are true:

(i) While the dynamics of such macroscopic systems are in principle reversible and periodic, in practice the time scale for this to occur can be exceedingly long, approaching the age of the universe. This is known as the Poincaré recurrence time.

So for all intents and purposes, the system can reach a "quasi steady state." Thus, for all intents and purposes a macroscopic system can reach an effective equilibrium

(ii) The entropy we care about is for the "macrostates." These states correspond to "coarse grained" cells in phase space

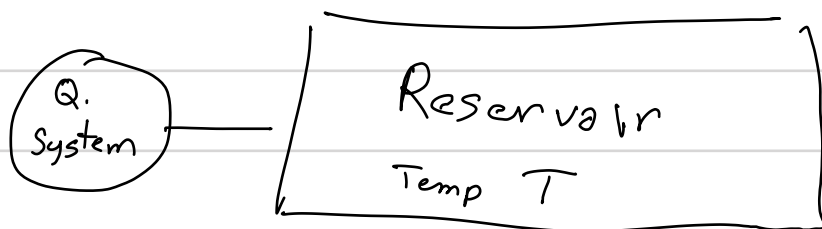
: Coarse grained delta: $\Delta(q-\tilde{q}, p-\tilde{p}) = 1$, $q = \tilde{q}$, $p = \tilde{p}$ in coarse grain

One can prove that the coarse grained entropy obeys the second law

(See e.g. E.T. Jaynes, Gibbs vs. Boltzmann Entropies, Am. J. Phys. 33 391 (1965).

These notions of entropy are associated with the microcanonical ensemble, a closed system with a well defined energy. The system itself is a macroscopic system with a number of degrees of freedom approach the

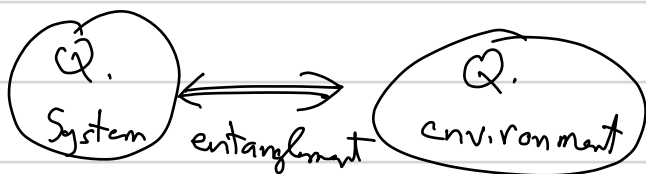
thermodynamic limit. In this course we will be concerned with a different limit where the system has few degrees of freedom, but the environment is a "reservoir" or "bath" at some temperature



This is the scenario of the canonical ensemble. The energy of the system is not conserved. We will see how in this open systems context the system (with few degrees of freedom) will come to thermodynamic equilibrium with the reservoir. The reservoir itself is a macroscopic system for which all of the notions of microcanonical entropy apply.

Decoherence

While the classical and quantum descriptions of open systems share many commonalities, there are some uniquely quantum phenomena. Most notably is entanglement. The quantum system can become entangled with the environment, a uniquely quantum correlation.

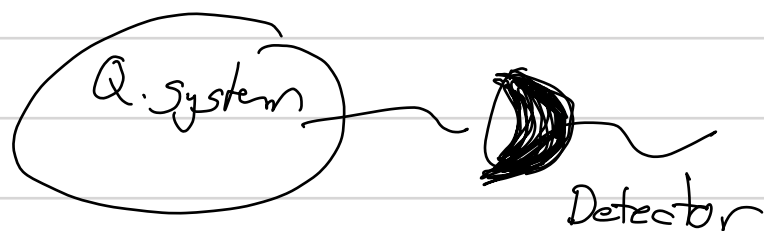


The entanglement between the system leads to "decoherence", the decay of quantum coherence - the ability to exhibit interference. Quantum system can exhibit superpositions of distinct states. In principle a cat can be in superposition of alive and dead - Schrödinger's cat! Why don't we see the effect of such superposition, i.e. interference of macroscopically distinct possibilities. The answer is decoherence

Decoherence is the loss of quantum coherence that arises because the system is coupled to the environment - it is an open system. And as we will see, the more macroscopic, and thus "nonclassical" the superposition is, the more fragile it is i.e. susceptible to decoherence. The loss of information associated with open quantum systems dynamics leads to a loss of quantum coherence, i.e. decoherence. Decoherence is essential in helping us to understand the quantum-to-classical transition, i.e., how the macroscopic world is well described by classical statistical physics, while the fundamental microscopic theory is quantum mechanics. Decoherence thus limits our ability to harness the unique properties of quantum systems for information processing. The fact that all quantum systems are open is the reason we don't have a quantum computer today. Understanding open quantum systems is thus interesting not only from a fundamental point of view, but also important for applications in quantum information processing.

Measurement

Another uniquely quantum feature is the role of measurement. In order for us to gain any information about a quantum system, we must measure it. Thus, when a quantum system is measured, it becomes an open quantum system



There is an intimate relationship between the dynamics of open quantum systems and quantum measurement. Of

course, there is the well known "measurement problem" in quantum mechanics - when we measure a quantum system we "collapse the wavefunction" and the appearance of randomness out of nowhere is not described but put in by hand. We want to solve this - no one has - but we will go a long way in understanding quantum measurement as a physical process and not a magical process (we'll hide the magic somewhere else :).