

Lecture 13

13 Decoherence I

A physical qubit is never isolated from its environment completely. As a trivial example, as in the case of a solid state qubit implementation, the physical qubit can be coupled directly to vibrations of its host lattice. It also can interact with the environment indirectly, as during gate operations through control fields. This interaction, even if it is weak, affects the dynamics of the qubit state and produces errors in quantum computation. Such errors do not have any analogue in classical computation. The initially-prepared, ideal state of a qubit eventually entangles with its environment after some time. Then, the quantum state cannot be described by a wave function for only a qubit. One must write a wave function for a whole system: qubit plus its environment. Such a wave function can have very complicated time dependence. So alternatively, one can use a density matrix representation. In the latter formalism a pure state of the qubit evolves to a mixed state due to decoherence, where the off-diagonal elements of the density matrix, coherences, decay to zero. In other words, the state loses its quantum interference property. The density matrix formalism [1, 2] is frequently used to describe the decoherence of quantum systems. However, one should understand the differences between the various types of averaging utilized by the density matrix formalism.

13.1 Density matrix

To describe the dynamics of a single isolated qubit you can use a wave function

$$|\psi(t)\rangle = a(t) |\uparrow\rangle + b(t) |\downarrow\rangle, \quad (1)$$

or a *pure* density matrix

$$\rho(t) = |\psi(t)\rangle \langle\psi(t)| = \begin{pmatrix} a(t)a^*(t) & a(t)b^*(t) \\ b(t)a^*(t) & b(t)b^*(t) \end{pmatrix}. \quad (2)$$

Then the evolution is described by a Schrödinger equation

$$i \left| \dot{\psi}(t) \right\rangle = H |\psi(t)\rangle, \quad (3)$$

or a Liouville-von Neumann equation

$$i\dot{\rho}(t) = [H, \rho]. \quad (4)$$

For an isolated quantum system these two representations are equivalent. Any expectation value of an operator \hat{A} can be written as $\langle A \rangle = \langle \psi(t) | \hat{A} | \psi(t) \rangle$ or $\langle A \rangle = \text{Tr} \{ \hat{A} \rho(t) \}$. The diagonal elements of the density matrix (2) provide probabilities for obtaining a spin-up or a spin-down qubit for a given quantum state. These are "quantum probabilities" that come from the probabilistic concept of quantum mechanics. Because quantum mechanics uses probability amplitudes rather than probabilities the off-diagonal elements of the density matrix, in general, are not zero. They describe quantum coherences between the up- and down-states.

Pure density matrix:

1. ρ is hermitian,
2. $\text{Tr} \{ \rho \} = 1$,
3. $\text{Tr} \{ \rho^2 \} = 1$.

You can parameterize the density matrix (2) using three expectation values $P_\alpha = \text{Tr} \{ \sigma_\alpha \rho \}$ of the Pauli matrices as (see lecture 2)

$$\rho(t) = \frac{1}{2} \begin{pmatrix} 1 + P_z & P_x - iP_y \\ P_x + iP_y & 1 - P_z \end{pmatrix}. \quad (5)$$

If there is an ensemble of qubits with different states and if you only know the probabilities p_k for particular states $|\psi_k\rangle$ then you can describe this ensemble by a set of wave functions

$$\begin{aligned} p_1 &: |\psi_1(t)\rangle, \\ p_2 &: |\psi_2(t)\rangle, \\ &\dots \\ p_n &: |\psi_n(t)\rangle, \end{aligned} \quad (6)$$

or by a *mixed* density matrix $\bar{\rho}(t)$ as

$$\bar{\rho}(t) = \sum_k p_k |\psi_k(t)\rangle \langle \psi_k(t)| = \sum_k p_k \begin{pmatrix} a_k(t)a_k^*(t) & a_k(t)b_k^*(t) \\ a_k(t)b_k^*(t) & b_k(t)b_k^*(t) \end{pmatrix}. \quad (7)$$

For a mixed density matrix $\text{Tr} \{ \rho^2 \} < 1$. The probabilities p_k are classical. They present our knowledge about the ensemble of quantum systems.

Both a pure and a mixed state can be represented as a vector of length $L \leq 1$ on a Bloch sphere. Moreover, a mixed state given by Eq. 6 also can be described by a set of Bloch vectors of unit length with a some probability distribution.

If a qubit ($s = \uparrow, \downarrow$) interacts with some other quantum system J then a wave function $|s, J\rangle$ should be used for the total system combining both the qubit and the system J . The equation of motion in this case is

$$i \frac{d}{dt} |s, J\rangle \langle s, J| = [H, |s, J\rangle \langle s, J|]. \quad (8)$$

We do not specify here a number of degrees of freedom for the system J . In general, it can be very large with small splitting between energy levels. In this case the system J is called a "bath". If you are not interested in dynamics of the system J , then you can project the total density matrix (wave function) to the states of a qubit only as

$$\begin{aligned}
\rho_{\uparrow\uparrow} &= \text{Tr} \{ |\uparrow\rangle \langle\uparrow| \rho \} = \sum_k \langle\uparrow, k| \rho |\uparrow, k\rangle, \\
\rho_{\uparrow\downarrow} &= \text{Tr} \{ |\uparrow\rangle \langle\downarrow| \rho \} = \sum_k \langle\downarrow, k| \rho |\uparrow, k\rangle, \\
\rho_{\downarrow\uparrow} &= \text{Tr} \{ |\downarrow\rangle \langle\uparrow| \rho \} = \sum_k \langle\uparrow, k| \rho |\downarrow, k\rangle, \\
\rho_{\downarrow\downarrow} &= \text{Tr} \{ |\downarrow\rangle \langle\downarrow| \rho \} = \sum_k \langle\downarrow, k| \rho |\downarrow, k\rangle.
\end{aligned} \tag{9}$$

The short notation for Eq. (9) is $\rho_s = \text{Tr}_J \{ \rho \}$, where ρ_s is a *reduced* density matrix. The reduced density matrix is pure only if the total wave function is a direct product of the wave functions of two subsystems $|s, J\rangle = |s\rangle \otimes |J\rangle$, which means that the subsystems are unentangled. In general, a reduced density matrix

$$\rho_s(t) = \begin{pmatrix} aa^* \langle J_\uparrow | J_\uparrow \rangle & ab^* \langle J_\downarrow | J_\uparrow \rangle \\ ba^* \langle J_\uparrow | J_\downarrow \rangle & bb^* \langle J_\downarrow | J_\downarrow \rangle \end{pmatrix}, \tag{10}$$

is mixed. One can add an additional statistical mixture here as an averaging over initial states of the system J . If the number of degrees of freedom in J is large and the splitting between energy levels is small, then it is difficult to determine the initial state. Frequently in this case, the initial state of the system is averaged over a distribution of initial bath states.

The coefficients $\langle J_m(t) | J_n(t) \rangle$ in Eq. (10) can be very complicated. The diagonal elements of the density matrix (10) have to be real non-negative numbers that sum up to one—because these are the probabilities. For the off-diagonal elements there are no such requirements except of the complex conjugation between $\rho_{\uparrow\downarrow}$ and $\rho_{\downarrow\uparrow}$. Usually, entanglement of a qubit with its environment leads to the decay of off-diagonal elements (this can be non-monotonic). This process is attributed to decoherence. However, if we use a basis where the initial state of the qubit is diagonal, then we do not have any decoherence. One has to use a specific basis (pointer states). Another way is to characterize the decoherence of a qubit by its entanglement with the environment or by how mixed is its final state. Frequently, long timescale decoherence can be described by a simple exponential decay. It will be shown in the following example.

13.2 Example I

Let's consider a simple model - a qubit coupled to the electromagnetic vacuum. We will solve it in the Wigner-Weisskopf approximation [3].

The Hamiltonian of the system is

$$H = -(\omega_0/2)\sigma_z + \sum_k \omega_k a_k^\dagger a_k + \sum_k (g_k a_k^\dagger \sigma^- + g_k^* a_k \sigma^+). \tag{11}$$

The initial state we start with is

$$|\psi(0)\rangle = (|-\rangle + |+\rangle) \otimes |0\rangle, \quad (12)$$

where $|0\rangle$ is the vacuum state of the electromagnetic field. Here we omit the normalization coefficient $\frac{1}{\sqrt{2}}$ for the sake simplicity. We assume that $|-\rangle$ is the ground state of the qubit and $|+\rangle$ is the excited state. The excited qubit state can emit a photon, while the ground state does not change in time. Then the wave function at time t can be written as

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}(\alpha(t)|+\rangle|0\rangle + |-\rangle|0\rangle + \beta(t)|-\rangle|1_k\rangle). \quad (13)$$

The qubit coherence terms $|+\rangle\langle-|$ and $|-\rangle\langle+|$ are proportional to $\alpha(t)$ and $\alpha^*(t)$ respectively. Therefore, $|\alpha(t)|$ describes decoherence of the qubit. Writing the Schrödinger equation with the Hamiltonian (11) and separating the coefficient at the orthogonal wave functions we get

$$\begin{aligned} |+\rangle|0\rangle : i\dot{\alpha}(t) &= \frac{\omega_0}{2}\alpha(t) + \sum_k g_k^* \beta_k(t), \\ |-\rangle|1_k\rangle : i\dot{\beta}(t) &= \frac{\omega_0}{2}\beta(t) + \omega_k \beta_k(t) + g_k \alpha(t). \end{aligned} \quad (14)$$

Using the Laplace transformation $\tilde{f}(s) = \int_0^\infty f(t)e^{-st}dt$ the system of differential eqns. (14) can be transformed to the linear system

$$\begin{aligned} iS\tilde{\alpha} - i &= \frac{\omega_0}{2}\tilde{\alpha} + \sum_k g_k^* \tilde{\beta}_k, \\ iS\tilde{\beta}_k &= -\frac{\omega_0}{2}\tilde{\beta}_k + \omega_k \tilde{\beta}_k + g_k \tilde{\alpha}, \end{aligned} \quad (15)$$

which easily transforms to the equation for $\tilde{\alpha}$

$$\tilde{\alpha} = \left\{ S + i \sum_k \frac{|g_k|^2}{iS + \omega_0 - \omega_k} \right\}^{-1}, \quad (16)$$

where $S = s + i\omega_0/2$. It is difficult to solve Eq. 16 exactly for the general case without apriori knowledge about the spectrum of the bath and the coupling coefficients. However, we can solve it for long times ($S \approx 0$) using the theory of residues. For details see Ref. [3]. Because all of the poles are simple we get the exponential decay

$$|\alpha(t)| \sim e^{-\Gamma t}. \quad (17)$$

We get that the relaxation of the qubit contributes to its decoherence. But this approximation is applicable for long timescales only.

One can derive [2, 3], for the general case of a quantum system coupled to a bath, that on long timescales coherences in the quantum system will decay exponentially. This derivation requires several crucial assumptions which cannot be applied to the short timescale evolution that is of interest in QC.

References

- [1] U. Fano, Rev. Mod. Phys. **29**, 74 (1957).
- [2] K. Blum, Density Matrix Theory and Applications, Plenum, New York, 1996.
- [3] W. H. Louisell, Quantum Statistical Properties of Radiation, Willey, New York, 1990.