

Lecture 14: Decoherence - introduction

QIC880, Adrian Lupascu

(Dated: 2013/10/25)

I. DENSITY MATRICES

The density matrix provides a description of a quantum system which generalizes the wavefunction representation. The density matrix is required for studying the dynamics of open quantum systems.

The density matrix can be introduced by analyzing the following situation. An ensemble (which can be provided either by a set of structure-wise identical quantum systems or by the repeated preparation of a single system) is prepared in the following way: states $|\psi_i\rangle$ are prepared with probabilities p_i ; proper normalization is assumed

$$\sum_i p_i = 1. \quad (1)$$

The expectation value of a operator A , which takes into account this uncertainty, is given by

$$\langle A \rangle = \sum_i p_i \langle \psi_i | A | \psi_i \rangle. \quad (2)$$

One can show that 2 is equal to

$$\langle A \rangle = \text{Tr}(\rho A) \quad (3)$$

with

$$\rho = \sum_i p_i |\psi_i\rangle \langle \psi_i|. \quad (4)$$

A different type of problem which requires the introduction of the density matrix appears when we consider the system S, with a Hilbert space spanned by the set $|i\rangle_S$ and the environment E with Hilbert space with basis set $|j\rangle_E$. A general quantum state of the system+environment is

$$\Psi = \sum_{ij} c_{ij} |i\rangle_S |j\rangle_E. \quad (5)$$

We want to calculate the expectation value of a operator A pertaining to the system. We have

$$\langle A \rangle = \langle \Psi | A \otimes I_E | \Psi \rangle = \sum_{ij} \sum_{kl} c_{ij} c_{kl}^* \langle l |_E \langle k |_S A \otimes I_E | i \rangle_S | j \rangle_E = \sum_j \langle \tilde{\psi}_j |_S A | \tilde{\psi}_j \rangle_S \quad (6)$$

where we introduced

$$|\tilde{\psi}_j\rangle_S = \sum_i c_{ij} |i\rangle_S. \quad (7)$$

The states above are in fact not normalized; we have

$$|\tilde{\psi}_j\rangle_S = \sqrt{p_j} |\psi_j\rangle_S \quad (8)$$

with $|\psi_j\rangle_S$ normalized and

$$p_j = \sum_i |c_{ij}|^2 \quad (9)$$

are such that their sum is unity (this follows from normalization of 5). The calculated value of A in 6 is thus of the same form as 3; the density matrix can thus be introduced as a way to describe the state of a system correlated with its environment.

The density matrix operator has the following properties:

- trace is unity

$$\text{Tr}(\rho) = 1. \quad (10)$$

- ρ is a positive operator, that is

$$\langle \phi | \rho | \phi \rangle \geq 0 \quad (11)$$

for any quantum state ϕ .

-

$$\text{Tr}(\rho^2) \leq 1 \quad (12)$$

with equality if the state is pure.

It is useful to use the following representation of ρ :

$$\rho = \frac{1}{2} (\text{I} + \mathbf{r} \cdot \boldsymbol{\sigma}) \quad (13)$$

where \mathbf{r} is a real vector and $\boldsymbol{\sigma}$ is a three-component "vector" with the three Pauli matrices as components:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad (14)$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad (15)$$

and

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (16)$$

This can be easily understood: any 2×2 matrix can be written as a linear combination of I , σ_x , σ_y , and σ_z ; the coefficients must be real for a Hermitian matrix, as the density matrix is. Finally the coefficient of I is given by asking for the trace to be one (note the other Pauli matrices are traceless).

It can be shown that

$$\text{Tr}(\rho^2) = \frac{1}{2}(1 + \mathbf{r}^2). \quad (17)$$

. Therefore one has

$$|\mathbf{r}| \leq 1 \quad (18)$$

with equality if and only if the state is pure. The following equalities are valid

$$r_i = \text{Tr}(\rho \sigma_i), i = \overline{1, 3}. \quad (19)$$

.

For a pure state, represented on the Bloch sphere as

$$|\psi\rangle = \cos \frac{\theta}{2} |0\rangle + \sin \frac{\theta}{2} e^{i\phi} |1\rangle \quad (20)$$

one has

$$r_x = \sin \theta \cos \phi, \quad (21)$$

$$r_y = \sin \theta \sin \phi, \quad (22)$$

and

$$r_z = \cos \theta. \quad (23)$$

It is justified to use therefore a representation of mixed states for a qubit on a sphere, where a mixed state is represented by the vector \mathbf{r} .

We next consider the evolution of the density matrix operator for a system evolving under its own Hamiltonian. The presence of an environment is not excluded (we can assume that this is what led to a mixed state in the first place), however we assume that the link to the environment is broken. We have

$$\rho(t) = \sum_i p_i |\psi_i(t)\rangle \langle \psi_i(t)| \quad (24)$$

from which

$$i\hbar \frac{d\rho}{dt} = [H, \rho]. \quad (25)$$

The time dependence of the density matrix can also be represented through a time dependent polarization vector $\mathbf{r}(t)$:

$$\rho(t) = \frac{1}{2} (\mathbf{I} + \mathbf{r}(t)\boldsymbol{\sigma}). \quad (26)$$

The Hamiltonian (which is in general time dependent) can be written as

$$H(t) = \frac{\hbar}{2} \boldsymbol{\omega}(t)\boldsymbol{\sigma}. \quad (27)$$

With 27 in 25 we find

$$\dot{\mathbf{r}}(t) = \boldsymbol{\omega}(t) \times \mathbf{r}(t). \quad (28)$$

The polarization vector precesses around the axis given by the effective field $\boldsymbol{\omega}(t)$ with an angular velocity given by the absolute value of this vector.

II. MODELS OF DECOHERENCE

In this section, we analyze two models of decoherence, as a mean to exemplify two types of manifestation of decoherence: energy relaxation (or T_1 processes) and pure dephasing (or T_2^* processes). We consider specific models of interaction between a two-level system and the environment in which an exact solution can be found. This is useful as a mean to build some intuition about how decoherence arises when a system is in contact with an environment, in particular how irreversible behaviour is generated due to the interaction with an environment.

A. Wigner-Weisskopf model for energy relaxation

We take a two level system with states $|g\rangle$ and $|e\rangle$, and an environment with many states, in particular with a large density of states for energies close to the transition frequency ω_{ge} of the system of interest (see Fig. 1).

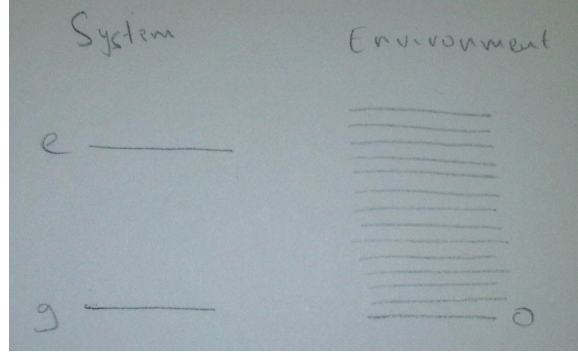


FIG. 1. Representation of the probability for a state \mathbf{k} to be occupied in the ground state.

We take the system to be initially in state $|e\rangle$ and the environment to be in the ground state. Given this situation and also the fact that the *rotating wave approximation* should hold, we can consider evolution in the manifold spanned by $|e, 0\rangle$ ($|0\rangle$ is the ground state of the environment) and the states $|g, k\rangle$ with k an index for the environment states. We denote $|e, 0\rangle$ by $|i\rangle$ (for initial) and $|g, k\rangle$ by $|k\rangle$. For this manifold the Hamiltonian is written as

$$H = H_0 + H_{int} \quad (29)$$

with

$$H_0 = \hbar\omega_{ge}|i\rangle\langle i| + \sum_k E_k|k\rangle\langle k| \quad (30)$$

and

$$H_{int} = \sum_k (W|k\rangle\langle i| + \text{hc}). \quad (31)$$

We can extract an energy offset ($\hbar\omega_{ge}$) and rewrite the Hamiltonian as

$$H = \sum_k \epsilon_k|k\rangle\langle k| + \sum_k (W|k\rangle\langle i| + \text{hc}). \quad (32)$$

with $\epsilon_k = E_k - \hbar\omega_{ge}$. We write the Schrodinger equation for the Hamiltonian 32 with a general wavefunction

$$\psi(t) = c_i(t)|i\rangle + \sum_k \lambda_k(t)e^{-i\frac{\epsilon_k}{\hbar}t}|k\rangle. \quad (33)$$

We obtain the following equations:

$$\dot{c}_i(t) = -i\frac{W}{\hbar} \sum_k \lambda_k(t)e^{-i\frac{\epsilon_k}{\hbar}t} \quad (34)$$

and

$$\dot{\lambda}_k(t) = -i \frac{W}{\hbar} e^{i \frac{\epsilon_k}{\hbar} t} c_i(t). \quad (35)$$

By integrating 35 we find

$$\lambda_k(t) = \frac{W}{i\hbar} \int_0^t dt' e^{i \frac{\epsilon_k}{\hbar} t'} c_i(t') \quad (36)$$

which is used in 34 to give

$$\dot{c}_i(t) = -\frac{W^2}{\hbar^2} \int_0^t dt' c_i(t') \sum_k e^{-i \frac{\epsilon_k}{\hbar} (t-t')}. \quad (37)$$

Let's consider that the energy levels of the environment are equally spaced, with space ϵ (a small quantity in the limit of a large environment) . We take

$$\epsilon_k = \epsilon(k - k_0) \quad (38)$$

with k_0 the index of the particular state of the environment which is closest to resonance to the two level system. The sum over k in 37 can be approximated by an integral in the limit when ϵ is very small. We have

$$\sum_k e^{-i \frac{\epsilon_k}{\hbar} (t-t')} = \frac{\hbar}{\epsilon} \sum_k \frac{\epsilon}{\hbar} e^{-i \frac{\epsilon_k}{\hbar} (t-t')} \approx \frac{\hbar}{\epsilon} \int d\omega e^{-i\omega(t-t')}. \quad (39)$$

We have

$$\int_{-\infty}^{\infty} d\omega e^{-i\omega(t-t')} = 2\pi \delta(t - t') \quad (40)$$

with $\delta(t - t')$ the Dirac delta function. If we use

$$\int_0^t dt' c_i(t') \delta(t - t') = c_i(t)/2 \quad (41)$$

in 37 we obtain a first order equation for c_i :

$$\dot{c}_i(t) = -\frac{\gamma}{2} c_i(t) \quad (42)$$

with

$$\gamma = \frac{2\pi W^2}{\hbar \epsilon} \quad (43)$$

The solution for 42 is

$$c_i(t) = e^{-\gamma t/2}, \quad (44)$$

so the probability of finding the system in the excited state decreases exponentially with rate γ . The final state at long times ($\gg \gamma^{-1}$) is "spread out" over a large number of states in the

environment. One can replace solution 44 in II A, and look at the probability of occupation of state k at long times. We find that only states within an energy window γ around the environment are occupied (however the probability to find any single environmental state is diluted due to the assumed large density of states).

The above solution indicates that energy is irreversibly lost to the environment. Is the system irreversible? We modeled it in fact using a Hamiltonian, and the time evolution is well defined. The system should exhibit recurrences which means that at long enough time the system should reach again the initial state. A very detailed discussion of this point, in particular a simple model for recurrent behavior, as well as useful pointers to literature, are given in [1].

Finally we discuss the connection of the Wigner-Weisskopf problem to results obtained using the Fermi's golden rule. The problem is the calculation of the transition probability from state $|i\rangle$ to state $|k\rangle$; these are eigenstates of the "main" part of the Hamiltonian (ie 30), with eigenstates E_i and E_k . In first order in perturbation theory the transition amplitude is given by

$$S_{ki} = \frac{1}{i\hbar} \int_0^t \langle k | H_{int} | i \rangle e^{i \frac{E_k - E_i}{\hbar} t} dt. \quad (45)$$

The transition probability from i to k is

$$P_{ki} = \frac{W^2}{\hbar^2} g_t(E_k - E_i) \quad (46)$$

where the function

$$g_t(E_k - E_i) = \text{sinc}^2 \left(\frac{(E_k - E_i)t}{\hbar} \right) t^2. \quad (47)$$

This function satisfies

$$\int_{-\infty}^{\infty} dE g_t(E) = 2\pi\hbar t. \quad (48)$$

When t is large enough this tends to a delta function in energy (the width of the function is \hbar/t), so the probability of transition is only significant in this energy interval.

If we now consider the case of many levels $|k\rangle$ we can find the total transition probability as an integral over the energy of the final state:

$$1 - P_i(t) = \int P_{ki}(E_k) D(E_k) dE_k \approx \frac{W^2}{\hbar^2} D(E_i) 2\pi\hbar t \quad (49)$$

In this approximation (which holds well when the probability of the initial state hasn't changed much, so its almost unity) we find a transition rate

$$\Gamma = \frac{W^2}{\hbar^2} D(E_i) 2\pi\hbar \quad (50)$$

This is the same as 43 if we take the density of states to be $1/\epsilon$.

The Wigner-Weisskopf model and the corresponding golden rule expression contain the generic features of energy relaxation for a system weakly coupled to an environment (in particular the proportionality with the square of the coupling factor and the proportionality with the energy density of states).

B. Models of dephasing

The Wigner-Weisskopf problem shows how decoherence shows up in the form of energy relaxation. Another type of decoherence can be considered, in which quantum information is lost without the energy being lost. We considered two different ways in which dephasing can occur.

1. Noise induced dephasing

Consider a two level system with hamiltonian

$$H(t) = \frac{\hbar\epsilon(t)}{2}\sigma_z, \quad (51)$$

with $\epsilon(t)$ a random variable with zero average. Note that in general the Hamiltonian may include as well a term proportional with σ_z of the form $\frac{\epsilon_0}{2}\sigma_z$ with ϵ_0 a constant; such a term can be removed if we move to the frame rotating around the z axis at frequency ϵ_0 . If we prepare a superposition $\alpha_0|0\rangle + \alpha_1|1\rangle$, after a time t this superposition becomes $\alpha_0 e^{-i\phi(t)/2}|0\rangle + e^{i\phi(t)/2}\alpha_1|1\rangle$ with the phase $\phi(t)$ given by

$$\phi(t) = \int_0^t dt' \epsilon(t'). \quad (52)$$

This phase is a random variable. Repeated runs of an experiment will lead to superpositions of $|0\rangle$ and $|1\rangle$ with different phase. On average the state becomes uncertain, thus decoherence occurs.

Note that decoherence occurs in a way which conserves the expectation value of σ_z , which we may associate with energy. Only phase is lost, for which reason this process is called "pure dephasing". The relevant operator to consider when evaluating this process is the expectation value of σ_x . This is given by

$$\langle\sigma_x(t)\rangle = \alpha_0^*\alpha_1\langle e^{i\phi(t)}\rangle + cc \quad (53)$$

When the time becomes long enough for the fluctuations of the phase $\phi(t)$ to become comparable with 2π , the system has completely lost its coherence, and the expectation value of σ_x vanishes; this time scale is the pure dephasing time.

2. Dephasing through interaction with a quantum bath

The model above was classical. We can also consider a quantum model of pure dephasing. We take the system prepared, as before, in state $\alpha_0|0\rangle + \alpha_1|1\rangle$. The bath is prepared in state $\sum_k \sqrt{p_k}|k\rangle$. We assume that the evolution of the system + environment after time t is given in the following way:

$$|0\rangle|k\rangle \rightarrow |0\rangle|k\rangle e^{-i\phi_k(t)/2} \quad (54)$$

and

$$|1\rangle|k\rangle \rightarrow |1\rangle|k\rangle e^{i\phi_k(t)/2}. \quad (55)$$

This evolution is allowed, as the transformation is unitary. .

$$\langle \sigma_x(t) \rangle = \alpha_0^* \alpha_1 \sum_k p_k e^{i\phi_k(t)} + cc. \quad (56)$$

In the above we can identify a factor similar to 53, namely

$$\langle e^{i\phi(t)} \rangle_{\text{quantum}} = \sum_k p_k e^{i\phi_k(t)}, \quad (57)$$

which will decay when we consider a large number of environmental states.

[1] M. Ligare and S. Becker, American Journal of Physics **63**, 788 (1995).

