Unitary Gate Control for Open Quantum Systems

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The annual progress seminar report entitled "Unitary Gate Control for Open Quantum Systems" submitted by Tejas Shetty (Roll No. 164120009) may be accepted for being evaluated.

Date: 29 January 2019

Prof. Sai Vinjanampathy

Declaration

I declare that this written submission represents my ideas in my own words and where others' ideas or words have been included, I have adequately cited and referenced the original sources. It also includes some of the results obtained through numerical calculations done by me. Some of the figures, used in this report, are schematically drawn by me while some are cited from other literature and the rest are plotted data obtained through numerical calculations. I declare that I have properly and accurately acknowledged all sources used in the production of this report. I also declare that I have adhered to all principles of academic honesty and integrity and have not misrepresented or fabricated or falsified any idea/data/fact/source in my submission. I understand that any violation of the above will be a cause for disciplinary action by the Institute and can also evoke penal action from the sources which have thus not been properly cited or from whom proper permission has not been taken when needed.

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Preliminaries

1.1 Jaynes Cummings Model

To better understand the Jaynes Cummings Model, it is instructive to consider the case of a single qubit or two level atom in a perfect non leaky cavity. (Gerry *et al.*, 2005)

Let the lower level be $|g\rangle$ and the upper level be $|e\rangle$. These two levels would be in contact with a electric field in the cavity. The cavity electric field in a quantized form is given by:

$$\hat{E} = \hat{e}\left(\frac{\hbar\Omega}{\epsilon_0 V}\right)^{1/2}(a_- + a_+)\sin(kz) \tag{1.1}$$

The interaction Hamiltonian would be the following format effectively.

$$H^{(I)} = -\hat{D}.\hat{E} \tag{1.2}$$

$$= dg\,(a_- + a_+) \tag{1.3}$$

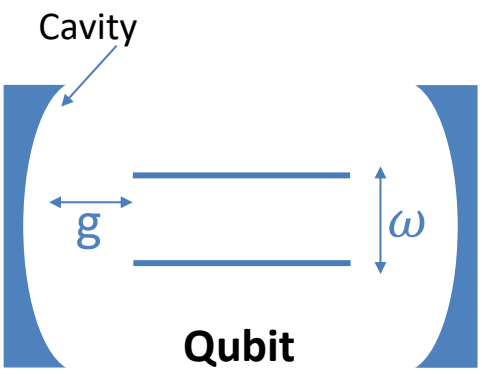


Figure 1.1: Single qubit in a perfect non leaky cavity

where d = dipole moment operator of the atom, $\hat{D}$ is the dipole moment vector,

$$g = -\left(\frac{\hbar\Omega}{\epsilon_0 V}\right)^{1/2} \sin(kz) \tag{1.4}$$

and $d = \hat{D}.\hat{e}$. At this point it is convenient to introduce the so-called atomic transition operators.

$$\sigma_+ = |e\rangle\langle g|, \quad \sigma_- = |g\rangle\langle e| = \sigma_+^\dagger, \tag{1.5}$$

and the inversion operator

$$\sigma_3 = |e\rangle\langle e| - |g\rangle\langle g|. \tag{1.6}$$

These operators obey the Pauli spin algebra

$$[\sigma_+, \sigma_-] = \sigma_3 \tag{1.7}$$

$$[\sigma_3, \sigma_\pm] = 2\sigma_\pm. \tag{1.8}$$

By parity, one can say that, the diagonal elements of $d = 0$. Symmetry conditions coerce an atom to have a net zero dipole movement, if it is in an energy eigenstate. Hence the diagonal elements of d would be zero $\langle e|d|e\rangle = 0 = \langle g|d|g\rangle$,

$$\begin{aligned} d &= d\,|g\rangle\langle e| + d^*\,|e\rangle\langle g| \\ &= d\sigma_- + d^*\sigma_+ = d(\sigma_+ + \sigma_-) \end{aligned} \tag{1.9}$$

where we have set $\langle e|d|g\rangle$ = d and have assumed, without loss of generality, that d is real. Thus the interaction Hamiltonian is

$$H^{(I)} = \hbar\lambda(\sigma_+ + \sigma_-)(a_- + a_+) \tag{1.10}$$

where $\lambda = dg/\hbar$

Derivation of the time dependence of the operators

The explanation below closely follows that in chapter 2, section 2.1 of (Gerry *et al.*, 2005). The Hamiltonian of a harmonic oscillator is given by

$$H = \hbar\Omega\left(a_+a_- + \frac{1}{2}\right) \tag{1.11}$$

The Heisenberg equation for operators reads as

$$\frac{dO}{dt} = \frac{i}{\hbar}[H, O] \tag{1.12}$$

On substituting for the annihilation operator a_- one gets

$$\begin{aligned}\frac{da_-}{dt} &= \frac{i}{\hbar}[H, a_-] \\ &= \frac{i}{\hbar}\left[\hbar\Omega\left(a_+a_- + \frac{1}{2}\right), a_-\right] \\ &= i\Omega\left(a_+a_-a_- - a_-a_+a_-\right) \\ &= i\Omega\left[a_-, a_+\right]a_- = -i\Omega a_-,\end{aligned} \tag{1.13}$$

which has the solution

$$a_-(t) = a_-(0)e^{-i\Omega t} \tag{1.14}$$

$$a_+(t) = a_+(0)e^{i\Omega t} \tag{1.15}$$

Another way of doing it would be via the Baker-Hausdroff lemma (Sakurai and Commins, 1995) For any two operators A and B,

$$e^{i\lambda A}Be^{-i\lambda A} = B + i\lambda[A, B] + \frac{(i\lambda)^2}{2!}[A[A, B]] + \ldots \tag{1.16}$$

The solution to (1.12) can be written as

$$O(t) = e^{iHt/\hbar}O(0)e^{-iHt/\hbar} \tag{1.17}$$

Applying it to (1.17) with a_- as H, λ as $t/\hbar$ and B as $O(0)$ we get,

$$\begin{aligned}O(t) = O(0) &+ \frac{it}{\hbar}[H, O(0)] \\ &+ \frac{1}{2!}\left(\frac{it}{\hbar}\right)^2[H, [H, O(0)]] + \ldots\ldots \\ &+ \frac{1}{n!}\left(\frac{it}{\hbar}\right)^n[H, [H, [H, \ldots. [H, O(0)]]]] + \ldots\ldots\end{aligned} \tag{1.18}$$

Replacing O by a_- one obtains

$$\begin{aligned}a_-(t) &= a_-(0)\left[1 - i\Omega t - \frac{\Omega^2t^2}{2!} + i\frac{\Omega^3t^3}{3!} + \ldots\ldots\right] \\ &= a_-(0)e^{-i\Omega t}\end{aligned} \tag{1.19}$$

Writing the evolution of operators once again,(just to avoid confusion)

$$a_-(t) = a_-(0)e^{-i\Omega t} \tag{1.20}$$

$$a_+(t) = a_+(0)e^{i\Omega t}$$

Similarly, the time evolution of the operators for the free-atomic case is as follows

$$\sigma_{\pm}(t) = \sigma_{\pm}(0)e^{\pm i\omega t} \tag{1.21}$$

expanding (1.10) we have

$$H^{(I)} = \hbar\lambda(\sigma_{+}a_{-} + \sigma_{+}a_{+} + \sigma_{-}a_{-} + \sigma_{-}a_{+}) \tag{1.22}$$

Let us look at approximate time dependencies for each of term in above mentioned equation. Using (1.21) and (1.20) one can compute the time dependence of each of the terms in the bracket in (1.22). Thus we can see that the approximate time dependences of the operator products in (1.22) are as follows:

$$\sigma_{+}a_{-} \sim e^{i(\Omega-\omega)t} \tag{1.23}$$

$$\sigma_{+}a_{+} \sim e^{i(\omega+\Omega)t} \tag{1.24}$$

$$\sigma_{-}a_{-} \sim e^{-i(\omega+\Omega)t} \tag{1.25}$$

$$\sigma_{-}a_{+} \sim e^{-i(\Omega-\omega)t} \tag{1.26}$$

If the electric field frequency in the cavity is not quite detuned from the spacing between the energy levels of the qubits then Ω is quite close to ω. Hence $\omega + \Omega$ is very much larger than $\omega - \Omega$ (because $\Omega \approx \omega$). On time averaging the Hamiltonian in (1.22) the contribution of the middle two terms becomes negligibly small if the above conditions hold. Since these terms oscillate very rapidly, on integration they get multiplied with a pre-factor which is quite huge as compared to first two terms. Hence they can be neglected. This approximation is also called as Rotating Wave Approximation (RWA). On carrying out RWA on (1.22) it transforms to

$$\hat{H}^{(I)} = \hbar\lambda(\sigma_{+}a_{-} + \sigma_{-}a_{+}) \tag{1.27}$$

1.2 Differential equation governing time evolution

1.2.1 Closed vs. open quantum systems

When one begins to learn quantum mechanics, it is implicitly assumed that all the systems that one studies exist in isolation. This is to say that they have no interaction with any other systems. In effect, all these system assumed to be closed and hence they are known as closed quantum systems. The system that we have here (i.e. two qubits in a leaky cavity) dissipates energy into the environment. Thus it is an open system in contrast to a closed one.

1.2.2 Need for density matrix formalism

Let us consider any arbitrary Hamiltonian H. Being an operator it would satisfy its eigenvalue equation [1]

$$H\,|m\rangle = E_m\,|m\rangle \tag{1.28}$$

Since the Hamiltonian is an energy operator the eigenvalues E_m are the energies of the eigenstates $|m\rangle$

$$E_m = \hbar\omega\left(m + \frac{1}{2}\right) \tag{1.29}$$

$$H = \frac{p^2}{2m} + \frac{m\omega^2}{2}x^2 \tag{1.30}$$

The energy eigenbasis is just a common one in which the Hamiltonian is written. One can also write it in the position basis. (Infinite dimension here we come) Just to have a feel of how different this representation is, let us calculate the probability $W(x)$ to find a particle in state $|m\rangle$ with energy E_m at position x is given by

$$W(x) = |\langle x\rangle\ m|^2 = |\varphi_m(x)|^2 \tag{1.31}$$

To consider the most general case let us assume that the wave function is in the linear combination of energy eigenstates.

$$|\psi\rangle = \sum_{m=0}^{\infty} c_m\,|m\rangle \tag{1.32}$$

This leads to

$$\begin{aligned}
\psi(x) &= \langle x\rangle\,\psi \\
&= \langle x|\left(\sum_{m=0}^{\infty} c_m\,|m\rangle\right) \\
&= \left(\sum_{m=0}^{\infty} c_m\langle x|\,|m\rangle\right) \\
&= \left(\sum_{m=0}^{\infty} c_m\,\langle x|\,|m\rangle\right) \\
&= \sum_{m=0}^{\infty} c_m\varphi_m(x)
\end{aligned} \tag{1.33}$$

Using this let us again try to calculate $W(x)$ to find the particle at position x:

[1] The treatment in this and the following three sections somewhat follows that in (Traxler, 2009)

$$\begin{aligned} W(x) &= |\langle x\rangle \psi|^2 = |\psi(x)|^2 \\ &= \varphi^*(x)\varphi(x) \\ &= \left(\sum_{m=0}^{\infty} c_m^* \varphi_m^*(x)\right)\left(\sum_{n=0}^{\infty} c_n \varphi_n(x)\right) \\ &= \sum_{m,n} c_m^* c_n \varphi_m^*(x)\,\varphi_n(x) \end{aligned} \tag{1.34}$$

Partitioning the sum in two parts, one in which the the indices are equal and one which they are not.

$$\begin{aligned} W(x) &= \sum_{m=0}^{\infty} |c_m|^2 |\varphi_m|^2 + \sum_{m\neq n} c_m^* c_n \varphi_m^*(x)\,\varphi_n(x) \\ &= \sum_{m=0}^{\infty} |c_m|^2 W_m + \sum_{m\neq n} c_m^* c_n \varphi_m^*(x)\,\varphi_n(x) \\ &= \sum_{m=0}^{\infty} p_m W_m(x) + \sum_{m\neq n} c_m^* c_n \varphi_m^*(x)\,\varphi_n(x) \end{aligned} \tag{1.35}$$

Where $|c_m|^2 = p_m$ is the probability to find the particle in m^{th} energy-eigenstate with the features $0 \leq p_m \leq 1$ and $\sum_m p_m = 1$ and $W_m = |\varphi_m|^2$ is the probability to find the m^{th} energy-eigenstate position x.

$$= \sum_{m=0}^{\infty} p_m W_m(x) + \sum_{m\neq n} c_m^* c_n \varphi_m^*(x)\,\varphi_n(x) \tag{1.36}$$

$$\sum_{m=0}^{\infty} + \sum_{m\neq n} \tag{1.37}$$

The first part $\sum_{m=0}^{\infty}$ is the sum of the probabilities of finding the particle in the m^{th} eigenstate times the probability to find the m^{th} eigenstate at position (x).

The second part $\sum_{m\neq 0}$ is the double sum of the off diagonal terms. The second part is what it imparts "quantumness" to quantum.

Digression

From Churchill and Brown (1990) any complex number can be expressed as either:

1. x+iy $(x, y \in \mathbb{R})$
2. r $e^{i\theta} (r, \theta \in \mathbb{R})$

where:

- x = real part
- y = imaginary part of the complex no
- r = modulus of the complex no
- θ = argument of the complex no or phases in physics and engineering .

For the sake of convenience, let us choose the 2^{nd} representation. Therefore one can write the expansion coefficients (of the wave function $|\psi\rangle$) c_m as

$$\begin{aligned} c_m &= \sqrt{p_m} e^{i\alpha_m} \\ c_m^* &= \sqrt{p_m} e^{i\alpha_m} \end{aligned} \tag{1.38}$$

where c_m is complex number, p_m is real number and α_m is an arbitrary phase.

c_m is a function of p_m , α_m. Let us say we have partial information about the state $|\psi\rangle$. If one knows c_m fully one can uniquely determine $|\psi\rangle$. In real life, one rarely has complete information about anything. One usually has to make do with what one has. Therefore it would not be right to assume that one has complete knowledge about the state $|\psi\rangle$. This implies, by virtue of what we had stated earlier that our knowledge of c_m too, is imperfect. This leads to the following possibilities:

- $\{p_m\}$ is not known
- $\{\alpha_m\}$ is not known
- we have partial knowledge of both $\{p_m\}$, $\{\alpha_m\}$

For reasons of pedagogy, time, space, etc. let us go ahead with option 2 i.e we have no idea about $\{\alpha_m\}$. Since we don't know $\{\alpha_m\}$ all the quantities we can measure are those in which any dependence over $\{\alpha_m\}$ is averaged away. To put it in another way any quantity that one calculates say z (p_m, α_m) we would have to find $\langle z \rangle_{\alpha_m}$ (or equivalently $\langle z \rangle_{phase}$ owing to our incomplete information.

An interesting thing to note in this connection is that

$$\left\langle e^{i\alpha_m} \right\rangle = \frac{1}{2\pi} \int_0^{2\pi} e^{i\alpha_m} d\alpha_m = 0 \tag{1.39}$$

coming back to (1.35) *we have*

$$
\begin{aligned}
W(x) &= \sum_{m}^{\infty} p_m W_m(x) + \sum_{m\neq n} c_m^* c_n \varphi_m^*(x)\varphi_n(x) \\
W(x) &= \sum_{m}^{\infty} p_m W_m(x) + \sum_{m\neq n} \sqrt{p_m} e^{-i\alpha_m} \sqrt{p_n} e^{i\alpha_n} \varphi_m^*(x)\varphi_n(x) \\
W(x) &= \sum_{m}^{\infty} p_m W_m(x) + \sum_{n\neq m} \sqrt{p_m}\sqrt{p_n} e^{i(\alpha_m-\alpha_n)} \varphi_m^*(x)\varphi_n(x) \qquad (1.40)
\end{aligned}
$$

On averaging we get:

$$
\begin{aligned}
\langle W(x)\rangle_{phase} &= \sum_{m=0}^{\infty} p_m W_m(x) \qquad (1.41) \\
&= \sum_{m=0}^{\infty} |c_m|^2 |\varphi_m|^2 \\
&= \sum_{m=0}^{\infty} |c_m|^2 |\varphi_m(x)|^2
\end{aligned}
$$

One can also go about getting $W(x)$ in an other way. Starting from (1.31)

$$
\begin{aligned}
W(x) &= |\langle x\rangle \psi|^2 \qquad (1.42) \\
\Big\langle W(x)\Big\rangle_{phase} &= \Big\langle |\langle x\rangle \psi|^2 \Big\rangle_{phase} \\
&= \Big\langle |\langle x|\ |\psi\rangle|^2 \Big\rangle_{phase} \\
&= |\langle x| \Big\langle |\psi\rangle \Big\rangle|^2_{phase}
\end{aligned}
$$

$$
\begin{aligned}
\langle|\psi\rangle\rangle_{phase} &= \frac{1}{2\pi}\int_0^{2\pi} |\psi\rangle\, d\alpha_m \\
&= \frac{1}{2\pi}\int_0^{2\pi} \sum_m \sqrt{p_m} e^{-i\alpha_m} |m\rangle\, d\alpha_m \\
&= \frac{1}{2\pi}\sum_m \sqrt{p_m}\Big(\int_0^{2\pi} e^{-i\alpha_m} |m\rangle\, d\alpha_m\Big)|m\rangle \\
&= \frac{1}{2\pi}\sum_m \sqrt{p_m} \times (0) \times |m\rangle \\
&= 0 \qquad (1.43)
\end{aligned}
$$

$$
\begin{aligned}
\therefore W(x) &= \Big|\langle x| \Big\langle |\psi\rangle \Big\rangle\Big|^2_{phase} \\
&= 0 \qquad (1.44)
\end{aligned}
$$

= a contradiction with (1.41) . Therefore this doesn't seem to be right. Some thing is wrong somewhere. Lets go back to (1.31) and start again. We had

$$\begin{aligned} W(x) &= |\langle x\rangle \psi|^2 \\ &= \langle x\rangle \psi \langle x\rangle \psi \\ &= \langle x\rangle \psi \langle \psi\rangle x \\ &= \langle x|\ |\psi\rangle \langle \psi|\ |x\rangle \end{aligned} \tag{1.45}$$

this can also be written as

$$\langle x|\ \underbrace{|\psi\rangle\langle\psi|}\ |x\rangle \tag{1.46}$$

where the quantity in the under brace

$$\langle x|\ \rho\, |x\rangle \tag{1.47}$$

is known as the density matrix. It is denoted by symbol ρ. Whenever one has incomplete information it is better to work with density matrix. Let us expand this quantity in terms of position basis

$$\begin{aligned} \rho = |\psi\rangle\langle\psi| &= \left(\sum_m c_m |m\rangle\right)\left(\sum_n c_n |n\rangle\right)^\dagger \\ &= \left(\sum_m c_m |m\rangle\right)\left(\sum_n (c_n |n\rangle)^\dagger\right) \\ &= \left(\sum_m c_m |m\rangle\right)\left(\sum_n |n\rangle^\dagger\, c_n^\dagger\right) \\ &= \left(\sum_m c_m |m\rangle\right)\left(\sum_n \langle n|\, c_n^*\right) \\ &= \sum_m c_m |m\rangle \sum_n \langle n|\, c_n^* \\ &= \sum_m \sum_n c_m |m\rangle \langle n|\, c_n^* \qquad (1.48) \\ &= \sum_m \sum_n c_m c_n^* |m\rangle \langle n| \qquad (1.49) \end{aligned}$$

Substituting from (1.38) we get

$$\begin{aligned} &= \sum_m \sum_n \sqrt{p_m} e^{i\alpha_m} \sqrt{p_n} e^{-i\alpha_n} |m\rangle\langle n| \\ &= \sum_m \sum_n \sqrt{p_m}\sqrt{p_n} e^{i\alpha_m} e^{-i\alpha_n} |m\rangle\langle n| \\ &= \sum_m \sum_n \sqrt{p_m}\sqrt{p_n} e^{i(\alpha_m-\alpha_n)} |m\rangle\langle n| \end{aligned} \tag{1.50}$$

One can also write it as

$$\rho = \sum_m p_m \left|m\right\rangle\!\left\langle m\right| + \sum_{n \neq m} \sqrt{p_m p_n} e^{i(\alpha_m - \alpha_n)} \left|m\right\rangle\!\left\langle n\right| \tag{1.51}$$

Averaging over all phases

$$\langle p \rangle_{phase} = \sum_m \rho_m \left|m\right\rangle\!\left\langle m\right| = \sum_m \rho_{mm} \left|m\right\rangle\!\left\langle m\right| \tag{1.52}$$

Using all this information in (1.47)

$$\begin{aligned}
\langle W(x) \rangle_{phase} &= \langle \langle x|\rho|x \rangle \rangle_{phase} && (1.53)\\
&= \langle x| \langle \rho \rangle_{phase} |x\rangle && (1.54)\\
&= \langle x| \left(\sum_m p_m \left|m\right\rangle\!\left\langle m\right| \right) |x\rangle && (1.55)\\
&= \sum_m p_m \langle x| \left(\left|m\right\rangle\!\left\langle m\right|\right) |x\rangle \\
&= \sum_m p_m \langle x\rangle\, m\, \langle m\rangle\, x \\
&= \sum_m p_m \langle x\rangle\, m\, \langle x\rangle\, m \\
&= \sum_m p_m |\langle x\rangle\, m|^2 \\
&= \sum_m p_m W_m(x) && (1.56)
\end{aligned}$$

Which is the correct answer (1.41) unlike (1.42)

Any density matrix is defined by (since information about phase is usually unknown)

$$\rho = \sum p_m \left|m\right\rangle\!\left\langle m\right| \tag{1.57}$$

$$|c_m|^2 = p_m = 1 \tag{1.58}$$

1.2.3 Properties of Density matrices

Positivity

$$\rho \geq 0 \tag{1.59}$$

Explanation :

Given any $|v\rangle$ $\langle v|\rho|v\rangle \geq 0$

The only condition is that $|v\rangle$ should not be a null vector.

Differently expressed

$$\begin{aligned}\langle\varphi|\rho|\varphi\rangle &= \langle\varphi| \sum_m p_m |m\rangle\langle m| |\varphi\rangle \\ &= \sum_m p_m \langle\varphi| |m\rangle\langle m| |\varphi\rangle \\ &= \sum_m p_m |\langle\varphi| m\rangle|^2 \geq 0 \end{aligned} \tag{1.60}$$

Self Adjoint

$$\rho = \rho^\dagger \tag{1.61}$$

The Adjoint of an operator $A = |\varphi\rangle\langle\psi|$ is

$$A^\dagger = (|\varphi\rangle\langle\psi|)^\dagger = (\langle\psi|)^\dagger (|\varphi\rangle)^\dagger = |\psi\rangle\langle\varphi| = |\psi\rangle\langle\varphi|$$

$$\rho^\dagger = \left(\sum_m p_m |m\rangle\langle m| \right)^\dagger \tag{1.62}$$

$$= \sum_m \left(p_m |m\rangle\langle m| \right)^\dagger \tag{1.63}$$

$$= \sum_m (|m\rangle\langle m|)^\dagger p_m^\dagger \tag{1.64}$$

$$= \sum_m (|m\rangle\langle m|)^\dagger p_m^* \tag{1.65}$$

$$= \sum_m p_m^* (|m\rangle\langle m|)^\dagger \tag{1.66}$$

$$= \sum_m p_m (|m\rangle\langle m|)^\dagger \tag{1.67}$$

($\because p_m \in \mathbb{R}$) since it is a probability

$$= \sum_m p_m (|m\rangle\langle m|)^\dagger \tag{1.68}$$

Unit trace

$$tr(\rho) = 1 \tag{1.69}$$

The trace of an operator A is as follows

$$tr(A) = \sum_i \langle i|A|i\rangle \tag{1.70}$$

$$\therefore tr(\rho) = \sum_i \langle i|\rho|i\rangle \tag{1.71}$$

$$= \sum_i \langle i| \left(\sum_m p_m |m\rangle\langle m| \right) |i\rangle \tag{1.72}$$

$$= \sum_i p_m \langle i\rangle m \langle m\rangle i \tag{1.73}$$

$$= \sum_i p_i = 1 \tag{1.74}$$

$\because$ sum of all probabilities add to 1

$$\rho^2 = \rho \tag{1.75}$$

$$\rho^2 = \rho \times \rho \tag{1.76}$$

$$= \left(\sum_m p_m |m\rangle\langle m| \right) \left(\sum_n p_n |n\rangle\langle n| \right) \tag{1.77}$$

$$= \sum_m \sum_n p_m p_n |m\rangle\langle m| |n\rangle\langle n| \tag{1.78}$$

$$= \sum_m \sum_n p_m p_n |m\rangle \delta_{mn} \langle n| \tag{1.79}$$

$$= \sum_m \sum_n p_m p_n \delta_{mn} |m\rangle\langle n| \tag{1.80}$$

$$= \sum_n p_n p_n |n\rangle\langle n| \tag{1.81}$$

$$= \sum_n p_n^2 |n\rangle\langle n| \tag{1.82}$$

$\sum_n p_n^2 |n\rangle\langle n| \neq \rho$ in general.

If $p_n = 1$ for $n = 1$ and $p_n = 0$ otherwise

then $\rho^2 = |1\rangle\langle 1|$ and $\rho = |1\rangle\langle 1|$.... $\therefore \rho^2 = \rho$

If $p_n = 1$ then the density ρ is a pure state otherwise it is a mixed state.

expectation value

The expectation value of an operator A is given as

$$\langle A\rangle = \langle\psi|A|\psi\rangle \tag{1.83}$$

$$tr(\rho A) = \sum_i \langle i|\rho A|i\rangle \tag{1.84}$$

$$= \sum_i \langle i|\left(\sum_m p_m \left|m\right\rangle\!\left\langle m\right| A\right)|i\rangle \tag{1.85}$$

$$= \sum_i \sum_m p_m \langle i\rangle\, m\, \langle m|A|i\rangle \tag{1.86}$$

$$= \sum_i \sum_m p_m\, \delta_{im}\, \langle m|A|i\rangle \tag{1.87}$$

$$= \sum_m p_m \langle m|A|m\rangle \tag{1.88}$$

$$= \sum_m |c_m|^2 \langle m|A|m\rangle \tag{1.89}$$

$$= \sum_m c_m c_m^* \langle m|A|m\rangle \tag{1.90}$$

$$= \sum_m \langle m|c_m^* A c_m|m\rangle \tag{1.91}$$

$$= \left(\sum_m \langle m|\, c_m^*\right) A \left(\sum_m c_m \left|m\right\rangle\right) \tag{1.92}$$

$$= \langle\psi|A|\psi\rangle = \langle A\rangle \tag{1.93}$$

$$\therefore\ tr(\rho A) = \langle A\rangle \tag{1.94}$$

1.2.4 Equation of Motion for density matrix

From Schroedinger's equation one has

$$i\hbar\frac{\partial}{\partial t}\left|\psi_i\right\rangle = H\left|\psi_i\right\rangle \tag{1.95}$$

Taking the complex conjugate we get

$$-i\hbar\frac{\partial}{\partial t}\langle\psi_i| = \langle\psi_i|\, H \tag{1.96}$$

Applying this equation for the density matrix we obtain:

$$i\hbar\frac{\partial}{\partial t}\rho = i\hbar\sum_i p_i\left(\left|\dot{\psi}_i\right\rangle\!\left\langle\psi_i\right| + \left|\psi_i\right\rangle\!\left\langle\dot{\psi}_i\right|\right)$$

$$= \sum_i p_i\left(H\left|\psi_i\right\rangle\!\left\langle\psi_i\right| - \left|\psi_i\right\rangle\!\left\langle\psi_i\right| H\right)$$

$$= H\rho - \rho H \tag{1.97}$$

Thus we obtain the Von Neumann-equation:

$$i\hbar\frac{\partial}{\partial t}\rho = [H,\rho] \tag{1.98}$$

1.2.5 A prelude to Lindblad master equation

The universe is always composed of our system of interest S and the environment E that it is in. Considering the total Hilbert space we get:

$$\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_E \tag{1.99}$$

The general form of Hamiltonian is:

$$H(t) = H_S \otimes \mathbb{1}_E + \mathbb{1}_S \otimes H_E + H_I(t) \tag{1.100}$$

where H_S is the Hamiltonian of the open system, H_E is the Hamiltonian of the environment and $H_I(t)$ denotes the interaction between system and environment. The operators which act exclusively on the system S are of the form

$$A \otimes \mathbb{1}_E \quad with \quad A \epsilon \mathcal{H}_S$$

We obtain density matrix of the system S by tracing over the environment. The expectation value of A is represented by:

$$\rho^S = tr_E(\rho) \tag{1.101}$$

$$\langle A\rangle = tr_S(\rho^S A) \tag{1.102}$$

Since the universe is a closed system it evolves unitary with time with the unitary responsible for it given by:

$$U(t,t_0) = Te^{-i\int_{t_0}^{t} H(t)dt} \tag{1.103}$$

Subjecting the universe density matrix to partial trace over the environment we get.

$$\rho^S(t) = tr_E\left(U(t,t_0)\,\rho(t_0)\,U^\dagger(t,t_0)\right) \tag{1.104}$$

Writing down the Von Neumann equation for a closed system we have:($\hbar = 1$)

$$\frac{\partial}{\partial t}\rho(t) = -i\left[H(t),\rho(t)\right],.$$

As explained before let us take a trace over the environment again

$$\frac{\partial}{\partial t}\rho^S(t) = -i\,tr_E\left([H(t),\rho(t)]\right) \tag{1.105}$$

Dynamical map, Operator sum representation, quantum dynamical semi-groups

Let us assume absence of initial correlations between the system and the environment. Hence the density operator can be described by a tensor product of ρ^S and ρ^E:

$$\rho(0) = \rho^S(0) \otimes \rho^E \tag{1.106}$$

$$\rho^S(0) \to \rho^S(t) = V(t)\rho^S(0) \equiv tr_E U(t,0)\rho^S(0) \otimes \rho^E U^t(t,0) \tag{1.107}$$

(where $V(t) : \mathcal{H}_S \to \mathcal{H}_E$ is called dynamical map.) (In the coming sections we will show that a dynamical map $V(t)$ can be completely characterized by operators acting on $\mathcal{H}_S$.) Writing down the spectral decomposition of ρ^E:

$$\rho^E = \sum_k p_k \; |\phi_k\rangle\langle\phi_k| \tag{1.108}$$

where $0 \leq p_k \, and \, \sum p_k = 1$.

Schematic diagram of the time evolution is as follows.

$$\rho(0) = \rho^S(0) \otimes \rho^E \to \underset{unitary\, time-evolution}{\overset{U(t,0)}{\longrightarrow}} \rho(t) = U(t,0)\rho^S(0) \otimes \rho^E U^\dagger(t,0) \tag{1.109}$$

$$\downarrow tr_E$$

$$\rho^S(0) \to \underset{dynamical\, map}{\overset{V(t)}{\longrightarrow}} \rho^S(t) = V(t)\rho^S(0) \tag{1.110}$$

For the density matrix of the universe we arrange for the following:

- at beginning $t = 0$ the density matrix is given as a product state:

$$\rho(0) = \rho^S(0) \otimes \rho^E \tag{1.111}$$

- at $t = 0$ the environment represents a pure state - it simplifies the discussions to a great extent

$$\rho^E(0) = |\phi_0\rangle\langle\phi_0| \tag{1.112}$$

Going back to (1.104) and making use of above inputs we have

$$\rho_{tot} \to U\rho^S(0) \otimes \rho^E U^\dagger \tag{1.113}$$

$$\Downarrow$$

$$\rho^S = tr_E\rho \to \sum_k \langle\phi_k| \, U\rho^S(0) \otimes |\phi_0\rangle\langle\phi_0| \, U^\dagger \, |\phi_k\rangle \tag{1.114}$$

(where $\{|\phi_k\rangle\}$ denote the complete states of the environment.)
Introducing Kraus - operators which live in the $\mathcal{H}_S$ Hilbert space

$$W_K =: \langle\phi_k| U |\phi_0\rangle \tag{1.115}$$

$$W_k^\dagger =: \langle\phi_0| U^\dagger |\phi_k\rangle \tag{1.116}$$

with the property

$$\sum_k W_k^\dagger W_k = \sum_k \langle\phi_0| U^\dagger |\phi_k\rangle \langle\phi_k| U |\phi_0\rangle = \langle\phi_0|U^\dagger U|\phi_0\rangle = \langle\phi_0|\mathbb{1}_{S+E}|\phi_0\rangle = \mathbb{1}_S \tag{1.117}$$

Thus the dynamical map of the time evolution of the density matrix of the system can be representation in terms of a sum of Kraus-operators:

$$\rho^S(0) \to \sum_k W_k \rho^S(0) W_k^\dagger = V\left[\rho^S(0)\right] = \rho^S(t) \tag{1.118}$$

Properties of the dynamical map $V(t)$:

- The dynamical map V (t) is trace conserving.

$$\begin{aligned}
tr_S\left(\rho^S(t)\right) &= tr_S\left(V\rho^S\right) \\
&= tr_S\left(\sum_k W_k \rho^S(0) W_k^\dagger\right) \\
&= \sum_k tr_S\left(W_k \rho^S(0) W_k^\dagger\right) \\
&= \sum_k tr_S\left(W_k^\dagger W_k \rho^S(0)\right) \because \text{cyclicity of trace} \\
&= tr_S\left(\sum_k W_k^\dagger W_k \rho^S(0)\right) \\
&= tr_S\left(\left(\sum_k W_k^\dagger W_k\right) \rho^S(0)\right) \\
&= tr_S\left(\mathbb{1}\,\rho(0)\right) \; from \; (1.117) \\
&= tr_S\left(\rho^S(0)\right)
\end{aligned} \tag{1.119}$$

- $V(t)$ is a convex linear map.

$$V(t) \sum_i p_i \rho_i = \sum_i p_i V(t) \rho_i, \tag{1.120}$$

$$\sum_i p_i = 1 \to \text{ convex sum} \tag{1.121}$$

- The dynamical map V (t) is completely positive.

$$V(t) \otimes 1_n \geq 0 \; \mathcal{H}_S \otimes \mathbb{C}^n \tag{1.122}$$

Let be a map $V(t)[\rho] \geq 0$ for all $\rho \geq 0$ and for all $t \geq 0$ on a finite dimensional complex Hilbert space. Then the map V is *completely positive* if the extension

$$V_n(t) = V(t) \otimes \mathbb{1}_n \tag{1.123}$$

$$V_n(t)\left[\rho \otimes \omega\right] = V(t)\left[\rho\right] \otimes \omega \geq 0 \tag{1.124}$$

for all $\rho \epsilon \mathcal{H}$ and for all $\omega \epsilon \mathbb{C}^n$

$V(t)$ is completely positive ,$\Leftrightarrow$ $V(t) \otimes V(t) \geq 0$ is positive.

This theorem is important for entangled systems, a counter example to complete positivity is the partial transposition.

Markovianity

If one assumes that the characteristic time scale of the environment τ_E is several orders of magnitude less than that of the system τ_S whatever excitations quantum information transferred to the environment is lost. quite fast as compared to the same process occurring in the system. The characteristic time scales are determined by some correlation functions proportional to $e^{-\frac{t}{\tau_E}}$ in case of the environment and $e^{-\frac{t}{\tau_S}}$ in case of the system.

This enables the dynamical map V to form a semi group:

$$V(t_1)V(t_2) = V\left(t_1 + t_2\right) \; where \, t_1, t_2 \geq 0 \tag{1.125}$$

The semi-group can be written in terms of its generators as :

$$V(t) = e^{\mathcal{L}t} \tag{1.126}$$

$$\Downarrow$$

$$\rho^S(t) = V(t)\rho^S(0) = e^{\mathcal{L}t}\rho^S(0) \tag{1.127}$$

The generator satisfies so-called master equation

$$\frac{\partial}{\partial t}\rho^S(t) = \mathcal{L}\rho^S\,(t) \tag{1.128}$$

where $\mathcal{L}$ is the so-called Liouville-operator.

1.2.6 Lindblad master equation

The aim of this section is to construct the most general form of the Liouville equation for a -finite dimensional complex Hilbert-space $\mathcal{H}_s$ with dim $\mathcal{H}_s = N^2$. our approach begins with constructing out of Kraus-operators an equation which contains the Hamilton-operator (plus remaining operators). This method goes back to Lindblad (1976) and to Gorini *et al.* (1976)

The master equation due to Lindblad is given by:

$$\frac{d}{dt}\rho^S(t) = -\frac{i}{\hbar}\left[H, \rho^S(t)\right] - D\left[\rho^S(t)\right] \tag{1.129}$$

where ρ^S is the density matrix of the system and $D\left[\rho^S\right]$ is the so-called dissipator

$$D[\rho^S] = \frac{1}{2}\sum_{k=1}^{N^2-1} \lambda_k \left(A_k^\dagger A_k \rho^S + \rho^S A_k^\dagger A_k - 2A_k \rho^S A_k^\dagger\right) \tag{1.130}$$

$$D[\rho^S] = \frac{1}{2}\sum_{k} \lambda_k \left(\left[A_k^\dagger, A_k \rho^S\right] + \left[\rho^S A_k^\dagger, A_k\right]\right) \tag{1.131}$$

with the Lindblad-operators A_k and the (positive) decoherence constants $\lambda_k \geq 0$ which are a quantitative measure for decoherence.

Assuming a weak coupling limit between the system and the environment

$$H \equiv H_{S+E} = H_S + H_E + H_{int} \tag{1.132}$$

for $H_E, H_{int} \to 0 \Rightarrow H = H_S$

Proof of the Lindblad-master-equation

Consider the dynamical map for the time-evolution of the density matrix of the system:

$$\rho^S \to V\left[\rho^S\right] = \sum_k W_k \rho^S W_k^\dagger \tag{1.133}$$

$$W_k = \langle \phi_k | U | \phi_0 \rangle \tag{1.134}$$

With the unitary operator $U = e^{-\frac{i}{\hbar}Ht}$ and the property $\sum_k W_k^\dagger W_k = 1$

The dynamical map fulfills the following properties:

- trace conserving
- convex linear
- completely positive

Some assumptions:

- The characteristic time scale of the system δt is much smaller than the lifetime of the system τ_S:

$$\delta t \ll \tau_S$$

- The environment should "forget" about the system, this is a so-called Markov process:

$$\tau_E \ll \delta t$$

Restarting from (1.133) keeping in mind the above assumptions taking into account.:

$$\rho^S(\delta t) = V\left[\rho^S(0)\right] = \sum_k W_k \rho^S(0) W_k^\dagger = \rho^S(0) + O(\delta t) \tag{1.135}$$

We see that the first Kraus-operator is of the order $\sim 1_S + O(\delta t)$, while all other Kraus-operators $\sim O(\delta t)$. are of the order of(δt)

$$W_0 = \mathbb{1}_S + \left(K - \frac{i}{\hbar} H\right)\delta t \tag{1.136}$$

$$W_k = A_k \sqrt{\delta t} \tag{1.137}$$

where K and H are hermitian operators and A_k is the Lindblad operator. From the normalization condition (1.117) we get:

$$\sum_k W_k^\dagger W_k = \mathbb{1}_S + \left(2K + \sum_k A_k^\dagger A_k\right)\delta t + O(\delta t^2) \tag{1.138}$$

$$\Downarrow$$

$$K = -\frac{1}{2}\sum A_k^\dagger A_k \tag{1.139}$$

Plugging the value of K back into (1.135) we get

$$\rho^S(\delta t) = W_0 \rho^S W_0^\dagger + \sum W_k \rho^S(0) W_k^\dagger =$$
$$= \left(\mathbb{1}_S + \left(K - \frac{i}{\hbar}H\right)\delta t\right)\rho^S(0)\left(\mathbb{1}_S + \left(K + \frac{i}{\hbar}H\right)\delta t\right) + \delta t \sum_k A_k \rho^S(0) A_k^\dagger = \quad (1.140)$$

Neglecting all higher order terms, we are left with

$$= \rho^S(0) + \delta t\{-\frac{i}{\hbar}\left[H, \rho^S(0)\right] - \frac{1}{2}\left(\sum A_k^\dagger A_k \rho^S(0) + \rho^S(0) A_k^\dagger A_k - 2A_k \rho^S(0) A_k^\dagger\right)\} \quad (1.141)$$

$$\Downarrow$$

$$\lim_{\delta t \to 0} \frac{\rho^S(\delta t) - \rho^S(0)}{\delta t} = \frac{d}{dt}\rho^S(t)|_{t=0} \qquad = -\frac{i}{\hbar}\left[H, \rho^S(t)\right]|_{t=0} - D\left[\rho^S(t)\right]|_{t=0} \quad (1.142)$$

Note: Here we have derived at $t = 0$ but it holds for any time and we have rescaled $A_k = \sqrt{\lambda_k} A_k$

Chapter 2

System Description and Previous work

2.1 Description of System

Qubits

A qubit is a quantum bit, the analog in quantum computing to the binary digit or bit of classical computing. Just as a bit is the basic unit of information in a classical computer, a qubit is the basic unit of information in a quantum computer. (Rouse, 2005)

In simple words, a qubit is a two level quantum mechanical system.

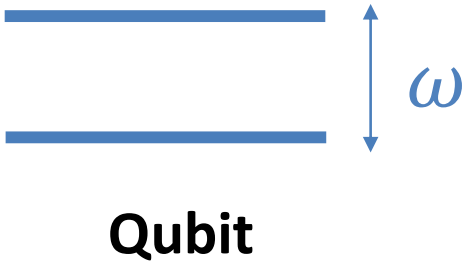


Figure 2.1: Qubit

Electromagnetic cavity

An electromagnetic cavity is an enclosure where standing electromagnetic waves can be sustained for considerable periods of time with or without an external driving field.

Figure 2.2: Cavity

Physics of system

To exemplify how state transfer could be enhanced by tweaking the underlying Hamiltonian it would be better to do so by means of trying it out on an actual physical system. The physical system (Shetty, 2017) that we choose for this purpose is as follows :

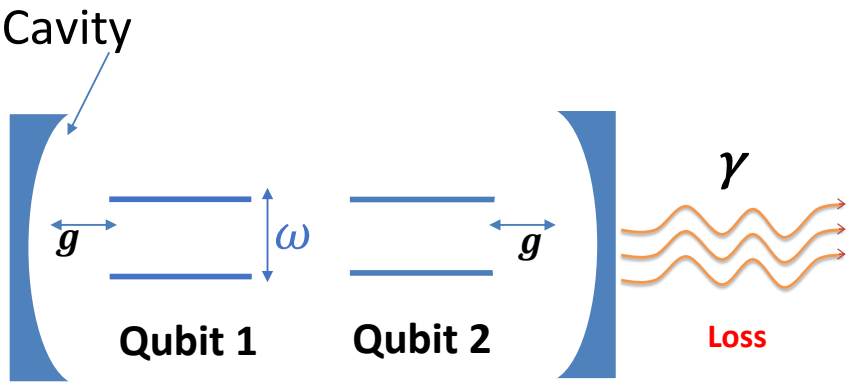


Figure 2.3: Two qubits in a leaky cavity

- We have:
  1. Two qubits each with an energy difference of ($\hbar\,\omega$).
  2. A single mode lossy cavity approximated as a harmonic oscillator with energy spacing of ($\hbar\,\Omega$).
- Dissipation of quantum information occurs at a characteristic rate (γ).
- There is no interaction between the qubits themselves.
- Both the qubits are coupled to the cavity
- The only way the qubits can communicate with each other is via the cavity

2.2 Hamiltonian of the system

The Hamiltonian of the system can be written as follows:

$$H = H_0 + V \tag{2.1}$$

where H_0 is the bare Hamiltonian and V is the coupling Hamiltonian. The bare Hamiltonian can be written as

$$H_0 = \frac{\omega}{2}\sigma_z \otimes I^{(2)} \otimes I^{(n)} + \frac{\omega}{2} I^{(2)} \otimes \sigma_z \otimes I^{(n)} + \Omega\, I^{(2)} \otimes I^{(2)} \otimes a_+ a_- \tag{2.2}$$

Where:

- ω = frequency corresponding to the energy spacing between the two levels of each qubit.
- Ω = frequency corresponding to the difference in the energy levels of the cavity.
- $\sigma_z, \sigma_+, \sigma_-$ = Pauli matrices.
- a_+, a_- = creation and annihilation operators for the cavity.
- $I^{(2)}$ is the identity in the qubit Hilbert space.
- $I^{(n)}$ is the identity in the harmonic oscillator Hilbert space.
- $\hbar$ is set to be equal to 1 in accordance with the usual practice.

In the above equation (2.2)

- The first part represents bare Hamiltonian for the qubit 1.
- The second part represents that of qubit 2.
- The third part represents that of cavity.

Now we will talk about how one would write down the interaction Hamiltonian V. Since, our system consists of qubits in a cavity effectively we have a double Jaynes Cummings type of Hamiltonian In our case since we have two qubits we will have two couplings, g_1 and g_2. g_1 is the parameter related to the strength of the coupling between the first qubit and the cavity. Similarly for g_2. So, following the discussion in the previous chapter we have

$$V = V_1 + V_2 \tag{2.3}$$

Where:

$$V_1 = g_1 \left(\sigma_- \otimes I^{(2)} \otimes a_+ \; + \; \sigma_+ \otimes I^{(2)} \otimes a_- \right) \tag{2.4}$$

$$V_2 = g_2 \left(I^{(2)} \otimes \sigma_- \otimes a_+ + I^{(2)} \otimes \sigma_+ \otimes a_- \right) \tag{2.5}$$

Putting all this together we get equation

$$V = g_1 \left(\sigma_- \otimes I^{(2)} \otimes a_+ \; + \; \sigma_+ \otimes I^{(2)} \otimes a_- \right) \; + \; g_2 \left(I^{(2)} \otimes \sigma_- \otimes a_+ + I^{(2)} \otimes \sigma_+ \otimes a_- \right) \tag{2.6}$$

Thus the full Hamiltonian is as follows:

$$\begin{aligned} H = \frac{\omega}{2} \sigma_z \otimes I^{(2)} \otimes I^{(n)} \; + \; \frac{\omega}{2} I^{(2)} \otimes \sigma_z \otimes I^{(n)} \; + \; \Omega \, I^{(2)} \otimes I^{(2)} \otimes a_+ a_- \\ + g_1 \left(\sigma_- \otimes I^{(2)} \otimes a_+ \; + \; \sigma_+ \otimes I^{(2)} \otimes a_- \right) \; + \; g_2 \left(I^{(2)} \otimes \sigma_- \otimes a_+ + I^{(2)} \otimes \sigma_+ \otimes a_- \right) \end{aligned} \tag{2.7}$$

Where all the symbols are as defined earlier and $\hbar$ is set to be equal to 1 in accordance with the usual practice.

Working of the system

This system works as follows:

- Qubit 1 is coupled to the cavity via the coupling Hamiltonian $g_1(\sigma_- \otimes I^{(2)} \otimes a_+ + \sigma_+ \otimes I^{(2)} \otimes a_-)$. Through these coupling the state of qubit 1 is being transferred to the cavity.
- Similar to qubit 1, qubit 2 is also coupled via the coupling Hamiltonian $g_2 \left(I^{(2)} \otimes \sigma_- \otimes a_+ + I^{(2)} \otimes \sigma_+ \otimes a_- \right)$. Through this coupling the information from the cavity is being transferred to qubit 2.
- All this while the cavity is also leaking quantum information at a rate γ.

2.2.1 Choice of Lindbladian operator

Having derived the Lindblad equation in the previous chapter it is time to decide what would be the Lindbladian operators. One thing that we know is they must be of the same dimensions, shape etc. as that of the density matrix. This is because both of them live in the Hilbert space of the system.

We know that the cavity is a leaky one i.e. it undergoes spontaneous emissions. The cavity has been modelled as a harmonic oscillator. On undergoing emission the oscillator drops down from one fock state to the one below it. This is equivalent to the action of a annihilation operator acting on the harmonic space oscillator.

Thus we can write

$$L = I^{(2)} \otimes I^{(2)} \otimes a_{-} \tag{2.8}$$

where all the terms are the same as defined before

2.2.2 Putting it all together

After all this hard work we end up with,

$$\frac{d\rho_s}{dt} = -i\,[H,\, \rho_s] + \gamma\left(L\,\rho_s\,L^{\dagger} - \frac{1}{2}\{L^{\dagger}\,L, \rho_s\}\right) \tag{2.9}$$

Where:

- ρ_s = Density matrix for the system which includes both the qubits and the cavity.
- Total Hamiltonian as written in (2.7)

$$H = \frac{\omega}{2}\,\sigma_z \otimes I^{(2)} \otimes I^{(n)} + \frac{\omega}{2}\,I^{(2)} \otimes \sigma_z \otimes I^{(n)} + \Omega\, I^{(2)} \otimes I^{(2)} \otimes a_{+}a_{-} + g\left(\sigma_{-} \otimes I^{(2)} \otimes a_{+} + \sigma_{+} \otimes I^{(2)} \otimes a_{-} + I^{(2)} \otimes \sigma_{-} \otimes a_{+} + I^{(2)} \otimes \sigma_{+} \otimes a_{-}\right)$$

  where we have additionally set g_1 equal to g_2 and replaced both of them by g, since this is the case which we could consider while performing the numerical calculations. Here g is the common coupling strength of the qubits to the cavity.

- $L = I^{(2)} \otimes I^{(2)} \otimes a_{-}$ Lindbladian operator as in (2.8)
- γ = Characteristic rate of dissipation for the cavity.
- $\hbar$ is set to be equal to 1 in accordance with the usual practice.

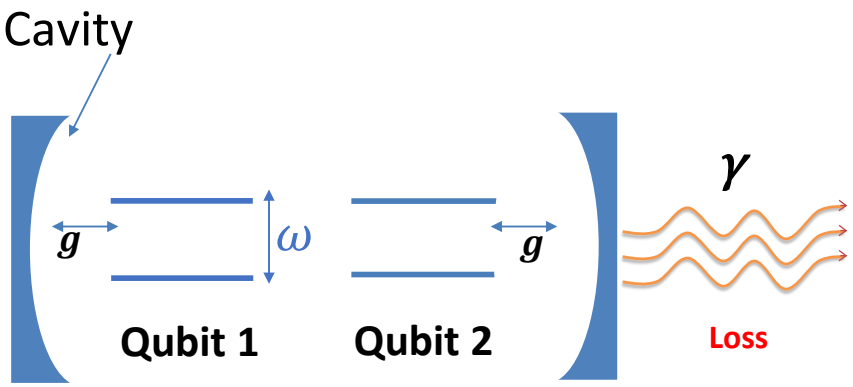
Chapter 3

Current progress

Recent developments in quantum dot based qubits have managed to convince us that good quality qubits are just around the corner. Mi *et al.* (2017) have managed to synthesize Si double quantum dot based qubits which have strong coupling between the single electron in the dot to the photonic field of a microwave cavity. This allows for entanglement and coupling over large distances. This enables us to envision devices which are quantum coupled or entangled with each other even if far away from each other.

Anyway coming back to the point, their set up is a double quantum dot qubit placed in a microwave cavity. This is quite similar to our setup in which we have two qubits place in a cavity.

The range of ω_c is about the range of ω_q. As we saw last time it is better to vary the field $g(t)$. Only if it is specific range and not otherwise looking for answers we hit upon Schuetz *et al.* (2017). By performing certain algebraic manipulations they manage to decouple the qubits from the cavity at specific intervals of time. The only way the qubits interact is via the cavity. If one moves the cavity there wont be any path by which they could decohere.This brings about long coherence times, and allows on to operate at "el-



evated temperatures" 1K to 4K. These temperatures are far higher than what one usually encounters in this field eg.mK. It also would allow us to make classical connections to quantum hardware.Here their system is exactly the same as ours but they require that the qubit level spacing ω_q is less than of ω_c. This puts it out of the range of Mi *et al.* (2017).

Basically we need a way in which one could efficiently develop control field temporal variation to implement a specific gate. It must be like an algorithm where on performing a series of steps either repeatedly or otherwise one ends up with a control field that performs the unitary we want. This it must be able to do to a tolerable (practical) level of error. Few of the algorithms that do this are:

- Krotov as in Tannor *et al.* (1992)
- Zhu and Rabitz (1998)
- GRAPE Khaneja *et al.* (2005)
- CRAB (Chopped RAndom Basis) Doria *et al.* (2011), Caneva *et al.* (2011)
- DCRAB (Dressed Chopped RAndom Basis) Rach *et al.* (2015)
- GOAT (Gradient Optimization of Analytic conTrols) Machnes *et al.* (2015)

Krotov (Tannor *et al.*, 1992) and (Zhu and Rabitz, 1998) were combined together in a single algorithm by (Maday and Turinici, 2003). GRAPE (Khaneja *et al.*, 2005) is Gradient Ascent by Pulse Engineering. It explicitly makes use of derivatives. When unable to do so it calculates a suitable thing which emulates them. Primarily they are gradient descent algorithms. They always get a solution but sometimes require appalling amount of computational resources. CRAB and its improvements DCRAB (Rach *et al.*, 2015) are basically non gradient methods which make use of analytic functions. These methods have may fail to reach the optimal solution but do so quickly on being successful.

GOAT (Machnes *et al.*, 2015) combines the best features of all before it to achieve high accuracy without compromising on speed. It is some what more complicated though.

To keep things simple lets start with Krotov by (Tannor *et al.*, 1992) algorithm in the form given by (Maday and Turinici, 2003). To gain deeper understanding, first we must generalize our system. So instead of

3.1 Introduction

Say, we want to apply a target unitary T_s on our quantum system. Let the Hamiltonian of our system be $\mathcal{H}$. The Lindbladian operators associated with it be $\{L_m\}$. The Hamiltonian

of the system is given by

$$H = H_0 + g(t)H_I \tag{3.1}$$

where,

H_0 : bare Hamiltonian

$g(t)$: control field as a function of time.

H_I : control Hamiltonian (interaction Hamiltonian)

The system is assumed to be governed by Lindblad equation.

$$\dot{\rho} = -i[H, \rho] + \mathcal{L}(\rho) \tag{3.2}$$

where,

$$\mathcal{L}(\rho) = \gamma \sum_k L_m \rho L_m^\dagger - 0.5\left\{L_m^\dagger L_m, \rho\right\}$$

The application of a target unitary T_s on the system can be translated in mathematical terms (in open quantum systems formalism) as follows :

$$\rho \rightarrow T_s \rho T_s^\dagger$$

So, the question at hand is what must be the form of $g(t)$ such that for any ρ if we let the system evolve (under the influence of the control field $g(t)$) we get the final state $T_s \rho T_s^\dagger$.

3.2 Taking advice from other sources

Suri *et al.* (2018) have discussed a similar problem with one major difference. Instead of implementing a specific unitary gate they have a fixed initial state which they wish to evolve to a fixed target state. They wish to find know how would $g(t)$ have to vary for the quantum system to evolve as close as possible to the target state. They discuss how this has already been done in many ways for closed quantum systems. The one which they focus upon is given in Reich *et al.* (2012).

Let us have quick review of it. Assuming we have a closed quantum system which we want to drive from a fixed state $|\psi_0\rangle$ to a target state $|\tau\rangle$. The Hamiltonian of the system is as in (3.1). For this the write down a cost function J as follows (details are in Suri *et al.* (2018)) :

$$J[|\psi\rangle, |\chi\rangle, g(t)] = \langle\psi(T)|Q|\psi(T)\rangle - 2Re\int_0^T dt\,\langle\chi(t)|\frac{d}{dt} + iH(t)|\psi(t)\rangle - \alpha\int_0^T dt g^2(t) \tag{3.3}$$

where $Q = |\tau\rangle\langle\tau|$. The first order variation J is set to zero to obtain a set of equations, namely

$$i\,|\dot{\psi}(t)\rangle = H(t)\,|\psi(t)\rangle\,, \text{with}\,|\psi(0)\rangle = |\psi_0\rangle \tag{3.4}$$

$$i\,|\dot{\chi}(t)\rangle = H(t)\,|\chi(t)\rangle\,, \text{with}\,|\chi(T)\rangle = Q\,|\psi(T)\rangle \tag{3.5}$$

$$g(t) = \frac{-1}{\alpha}\mathrm{Im}\,\langle\chi(t)|\mu|\psi(t)\rangle \tag{3.6}$$

Following Reich *et al.* (2012), Eqns. (3.4) could be solved self-consistently as below,

$$i\,|\dot{\psi}^{(k)}(t)\rangle = H^{(k)}(t)\,|\psi^{(k)}(t)\rangle\,, \text{with}\,|\psi^{(k)}(0)\rangle = |\psi_0\rangle \tag{3.7}$$

$$i\,|\dot{\chi}^{(k)}(t)\rangle = H^{(k)}(t)\,|\chi^{(k)}(t)\rangle\,, \text{with}\,|\chi^{(k)}(T)\rangle = Q\,|\psi^{(k)}(T)\rangle \tag{3.8}$$

$$g^{(k)}(t) = (1-\delta)\tilde{g}^{(k-1)}(t) - \frac{\delta}{\alpha}\mathrm{Im}\left\langle\chi^{(k-1)}(t)\middle|\mu\middle|\psi^{(k)}(t)\right\rangle \tag{3.9}$$

$$g^{(k)}(t) = (1-\eta)\tilde{g}^{(k)}(t) - \frac{\delta}{\alpha}\mathrm{Im}\left\langle\chi^{(k)}(t)\middle|\mu\middle|\psi^{(k)}(t)\right\rangle \tag{3.10}$$

For open quantum systems Suri *et al.* (2018) suggest to move from the Hilbert space to Liouville space, which involves vectorizing the density matrix ρ as $|\psi\rangle\rangle$. So the problem goes from

$$\rho_0 \rightarrow \rho_f \tag{3.11}$$

$$\dot{\rho} = -i[H,\rho] + \gamma\sum_k\left(L_m\rho L_m^\dagger - 0.5\left\{L_m^\dagger L_m,\rho\right\}\right) \tag{3.12}$$

$$\text{to,}\ |\psi_0\rangle\rangle \rightarrow |\tau\rangle\rangle \tag{3.13}$$

$$i\,|\dot{\psi}(t)\rangle\rangle = A(t)\,|\psi(t)\rangle\rangle,\ \text{where} \tag{3.14}$$

$$A(t) = I\otimes H(t) - H^*(t)\otimes I + i\gamma\sum_k\left(L_m^T\otimes L_m - 0.5\left(I\otimes L_m^\dagger L_m + L_m^T L_m^*\otimes I\right)\right) \tag{3.15}$$

3.3 Back to our problem

Coming to our problem we have,

$$\rho \rightarrow T_s\rho T_s^\dagger \tag{3.16}$$

$$\dot{\rho} = -i[H,\rho] + \gamma\sum_k\left(L_m\rho L_m^\dagger - 0.5\left\{L_m^\dagger L_m,\rho\right\}\right) \tag{3.17}$$

Moving to Liouville space one can rewrite it as,

$$|\psi\rangle\rangle \rightarrow T_s^T\otimes T_s\,|\psi\rangle\rangle \tag{3.18}$$

$$i\,|\dot{\psi}(t)\rangle\rangle = A(t)\,|\psi(t)\rangle\rangle \tag{3.19}$$

where $A(t)$ is as given before in equation (3.11). From now on wards, let $T_s^T\otimes T_s$ be called as T. But unlike Suri *et al.* (2018) instead of initial and final states we have the target unitary T. So, we cannot write the same cost function and optimize it to get the desired control field.

3.4 Putting it all together

Since,

$$i\,|\dot{\psi}(t)\rangle\rangle = A(t)\,|\psi(t)\rangle\rangle \tag{3.20}$$

$$|\psi(t)\rangle\rangle = \mathcal{T}\left(e^{-i\int_0^T dtA(t)}\right)|\psi(0)\rangle \tag{3.21}$$

where $\mathcal{T}$ is the time ordering operator. Let $\mathcal{T}\left(e^{-i\int_0^T dtA(t)}\right)$ be denoted by $\mathcal{L}$. One can approximate it as follows:

$$\mathcal{L} = \mathcal{T}\left(e^{-i\int_0^T dtA(t)}\right) \tag{3.22}$$

$$\mathcal{L} = \prod_{k=N}^{1} \mathcal{L}_k \tag{3.23}$$

$$\tag{3.24}$$

where $\mathcal{L}_k = e^{-iA(t_k)\delta t}$. Let us define a few other terms.

$$\mathcal{L}_k^d = \mathcal{L}_N\mathcal{L}_{N-1}\ldots X_k\mathcal{L}_k\ldots\mathcal{L}_2\mathcal{L}_1 \tag{3.25}$$

$$X_k = I\otimes H_I(t) - H_I^*(t)\otimes I \tag{3.26}$$

Now we shall define $F[g] = -Tr((T-\mathcal{L})^\dagger(T-\mathcal{L}))$ to be our fidelity measure as in Khaneja *et al.* (2005). Next we need to devise an update step for the control field which would improve the fidelity. Following Khaneja *et al.* (2005) we have

$$g(t_{k+1}) = g(t_k) + \epsilon\frac{\partial F}{\partial g(t_k)}, \text{ or} \tag{3.27}$$

$$g_{k+1} = g_k + \epsilon\frac{\partial F}{\partial g_k} \tag{3.28}$$

ϵ is constant which would depend on the speed at which one would want to converge,etc.

$$\frac{\partial F}{\partial g_k} = -Tr((T-\frac{\partial\mathcal{L}}{\partial g_k})^\dagger(T-\mathcal{L})) - Tr((T-\mathcal{L})^\dagger(T-\frac{\partial\mathcal{L}}{\partial g_k})) \tag{3.29}$$

$$\frac{\partial F}{\partial g_k} = -Tr((T-\mathcal{L}_k^d)^\dagger(T-\mathcal{L})) - Tr((T-\mathcal{L})^\dagger(T-\mathcal{L}_k^d))) \tag{3.30}$$

$$\mathcal{L}_k^d = \frac{\partial\mathcal{L}}{\partial g_k} = \frac{\partial(\mathcal{L}_N\mathcal{L}_{N-1}\ldots\mathcal{L}_k\ldots\mathcal{L}_2\mathcal{L}_1)}{\partial g_k} \tag{3.31}$$

$$\mathcal{L}_k^d = \frac{\partial\mathcal{L}}{\partial g_k} = \mathcal{L}_N\mathcal{L}_{N-1}\ldots\frac{\partial\mathcal{L}_k}{\partial g_k}\ldots\mathcal{L}_2\mathcal{L}_1 \tag{3.32}$$

$$\mathcal{L}_k^d = \mathcal{L}_N\mathcal{L}_{N-1}\ldots X_k\mathcal{L}_k\ldots\mathcal{L}_2\mathcal{L}_1 \tag{3.33}$$

$$X_k = I\otimes H_I(t) - H_I^*(t)\otimes I \tag{3.34}$$

3.4.1 Steps to find optimal control field

1. Start with a random $g_{rand}(t)$.
2. Calculate fidelity F.
3. Update $g(t)$ using Equation (3.27)
4. If fidelity F calculated from new $g(t)$ differs from old one by more than μ, then go to step 3.
5. Terminate.

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