# Open quantum systems: part-II

Jukka Pekola[1] and Bayan Karimi[1]
[1]Pico group, QTF Centre of Excellence, Department of Applied Physics, Aalto University School of Science
(Dated: November 16, 2020)

## I. PREREQUISITES

Liouville - von Neumann equation follows mechanically from the Schrödinger equation as follows. First, in the Schrödinger picture we have

$$i\hbar\partial_t|\psi(t)\rangle = H|\psi(t)\rangle \tag{1}$$

for a state $|\psi(t)\rangle$ and Hamiltonian $H$. We can write the solution of it formally as

$$|\psi(t)\rangle = U(t,t_0)|\psi(t_0)\rangle, \tag{2}$$

where $U(t,t_0)$ is the time evolution operator between the initial time $t_0$ and $t$. It then obeys

$$i\hbar\partial_t U(t,t_0) = HU(t,t_0). \tag{3}$$

The density matrix of the whole system can be written as

$$\rho_S(t) = \sum_\lambda p_\lambda|\psi_\lambda(t)\rangle\langle\psi(t)|, \tag{4}$$

where $p_\lambda$ are the (positive) weights for the states $|\psi_\lambda(t)\rangle$ that obey the Schrödinger equation. We then find

$$\rho_S(t) = \sum_\lambda p_\lambda U(t,t_0)\rho_S(t_0)U^\dagger(t,t_0). \tag{5}$$

Using the chain rule in differentiating, we then find easily that

$$\dot\rho_S(t) = \frac{i}{\hbar}[\rho_S(t), H], \tag{6}$$

which is the Liouville - von Neumann equation.

It is, however, often useful to employ the corresponding equation in the interaction picture, where operators (including the density operator) obey

$$A_I(t) = e^{iH_0t/\hbar}A_S e^{-iH_0t/\hbar}. \tag{7}$$

Here $H_0$ is the unperturbed Hamiltonian, and $H = H_0 + V$ with $V$ as the interaction. Then by a straightforward calculation we find that

$$\dot\rho_I(t) = \frac{i}{\hbar}[\rho_I(t), V_I(t)]. \tag{8}$$

## II. MASTER EQUATIONS FOR DISSIPATIVE QUANTUM CIRCUITS

### A. Second-order master equation

We aim to write the master equation for reduced density matrix of an open quantum system. The standard way is to write total density matrix in the weak coupling regime as a product $\rho_{\rm tot} = \rho\otimes\rho_{\rm B}$, where $\rho$ and $\rho_{\rm B}$ are the density matrix of the system and environment, respectively. For simplicity we write $\rho_{\rm tot} = \rho\rho_{\rm B}$. The Liouvillevon Neumann equation in the interaction picture then reads

$$\dot\rho_{\rm tot}(t) = \frac{i}{\hbar}[\rho_{\rm tot}(t), V_I(t)]. \tag{9}$$

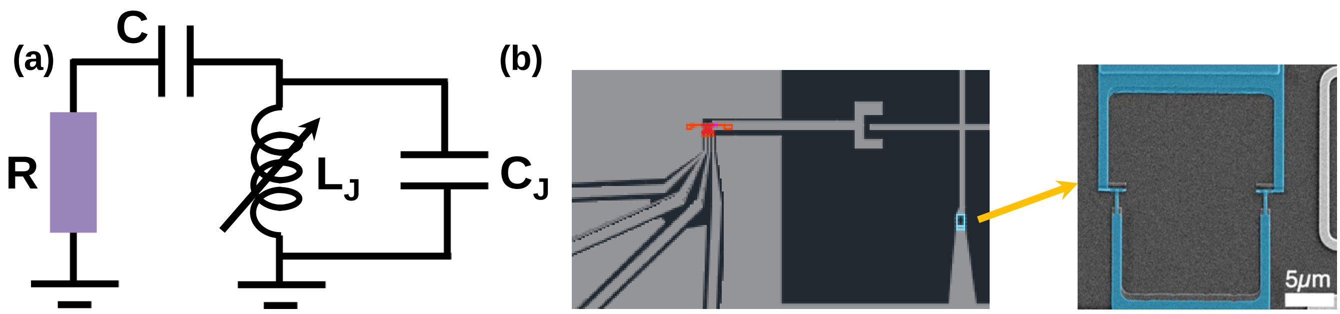


FIG. 1: Exemplary quantum circuit for analysis. (a) Circuit diagram. On the right side a SQUID (superconducting quantum interference device) composed of two Josephson junctions. This element is capacitively coupled to a resistive element on the left. (b) The actual on-chip circuit. The coupling capacitor is the fork-like structure in the middle, and the SQUID is zoomed out in blue on the right. The resistive element is contacted by four NIS tunnel junctions to control and measure temperature, on the left.

If we switch on the interaction at time $t$, the total density matrix $\rho_{\rm tot}$ is

$$\rho_{\rm tot}(t) = \rho_{\rm tot}(-\infty) + \int_{-\infty}^{t} dt' \dot{\rho}_{\rm tot}(t') \tag{10}$$

Substituting this equation in Eq. (9) we have

$$\begin{aligned} \dot{\rho}_{\rm tot}(t) &= \frac{i}{\hbar}[\rho_{\rm tot}(-\infty), V_I(t)] + \int_{-\infty}^{t} dt' [\dot{\rho}_{\rm tot}(t'), V_I(t)] & (11)\\ &= \frac{i}{\hbar}[\rho_{\rm tot}(-\infty), V_I(t)] - \frac{1}{\hbar^2}\int_{-\infty}^{t} dt' \big[[\rho_{\rm tot}(t'), V_I(t')], V_I(t)\big]. & (12)\end{aligned}$$

Taking into account that $\rho_{\rm B}$ represents the density matrix of an infinite bath that does not change with time, Eq. (11) will be

$$\dot{\rho}(t)\rho_{\rm B} = \frac{i}{\hbar}[\rho(-\infty)\rho_{\rm B}, V_I(t)] - \frac{1}{\hbar^2}\int_{-\infty}^{t} dt' \big[[\rho(t')\rho_{\rm B}, V_I(t')], V_I(t)\big]. \tag{13}$$

In order to see the density matrix of the system only, not the one of the bath, we take a trace over bath ($\mathrm{Tr_B}$) from the above equation

$$\dot{\rho}(t) = \mathrm{Tr_B}\big\{\frac{i}{\hbar}[\rho(-\infty)\rho_{\rm B}, V_I(t)]\big\} - \frac{1}{\hbar^2}\mathrm{Tr_B}\big\{\int_{-\infty}^{t} dt' \big[[\rho(t')\rho_{\rm B}, V_I(t')], V_I(t)\big]\big\}, \tag{14}$$

where we used $\dot{\rho}(t) = \mathrm{Tr_B}\{\dot{\rho}(t)\rho_{\rm B}\}$.

### B. Exemplary system under study

Now we will solve Eq. (14) and obtain the density matrix for a real system shown in Fig. 1. The total Hamiltonian of the system and the environment reads

$$H_0 = H_S + V(t) + H_B, \tag{15}$$

where $H_s = \hbar\omega_0 a^\dagger a$ is the Hamiltonian of the system, dc-SQUID, with creation and annihilation operators $a^\dagger$, $a$, respectively, $V(t) = i\lambda(a - a^\dagger)$ denotes the coupling between the system and voltage noise source of the bath $Qv_n(t)$ (perturbation), and finally $H_B$ is the Hamiltonian of the environment here mainly the heat bath (resistor with resistance $R$). The perturbation in the interaction picture is given by

$$V_I(t) = i\gamma e^{iH_0t/\hbar}(a - a^\dagger)e^{-iH_0t/\hbar}v_n(t), \tag{16}$$

where $\gamma = \lambda\sqrt{\frac{\hbar}{2Z_0}} = \frac{C}{C+C_J}\sqrt{\frac{\hbar}{2Z_0}}$ for the system shown in Fig. 1(a), and $Z_0 = \sqrt{\frac{L_J}{C_J}}$.

The resulting master equation reads

$$\dot{\rho}_{gg}(t) = -\Gamma_\uparrow \rho_{gg} + \Gamma_\downarrow \rho_{ee} \tag{17}$$

$$\dot{\rho}_{ge}(t) = -\frac{1}{2}(\Gamma_\downarrow + \Gamma_\uparrow)\rho_{ge}, \tag{18}$$

where the excitation and relaxation rates are $\Gamma_\uparrow = \frac{\gamma^2}{\hbar^2} S_v(-\omega_0)$ and $\Gamma_\downarrow = \frac{\gamma^2}{\hbar^2} S_v(\omega_0)$, respectively.

The derivation for diagonal element Eq. (17) will be presented in detail on the lecture.

## III. NOISE OF TUNNELING

As we mentioned in the previous lecture (Lecture-6EXP), in order to calculate noise of, for example, tunneling, one needs to evaluate

$$S_{\dot{N}_L}(\omega) = \int_{-\infty}^{\infty} dt\; e^{i\omega t} \langle \dot{N}_L(t)\dot{N}_L(0)\rangle, \tag{19}$$

where $\dot{N}_L$ is the particle current operator, Eq. (4) in Lecture-4EXP, which was given by

$$\dot{N}_L = \frac{i}{\hbar}\sum_{l,r}(t_{rl} a_r^\dagger a_l - t_{lr} a_l^\dagger a_r). \tag{20}$$

The first task is to calculate the two-time correlator $\langle \dot{N}_L(t)\dot{N}_L(0)\rangle$. In the interaction picture Eq. (20) reads

$$\dot{N}_L(t) = \frac{i}{\hbar}\sum_{l,r}(t_{rl} a_r^\dagger a_l e^{i(\epsilon_r-\epsilon_l)t/\hbar} - t_{lr} a_l^\dagger a_r e^{-i(\epsilon_r-\epsilon_l)t/\hbar}). \tag{21}$$

Then we have

$$\langle \dot{N}_L(t)\dot{N}_L(0)\rangle = -\frac{1}{\hbar^2}\sum_{l,r,l',r'} \langle (t_{rl} a_r^\dagger a_l e^{i(\epsilon_r-\epsilon_l)t/\hbar} - t_{lr} a_l^\dagger a_r e^{-i(\epsilon_r-\epsilon_l)t/\hbar})(t_{r'l'} a_r'^\dagger a_l' - t_{l'r'} a_l'^\dagger a_r')\rangle. \tag{22}$$

Again only $l = l'$ and $r = r'$ terms survive:

$$\begin{aligned}\langle \dot{N}_L(t)\dot{N}_L(0)\rangle &= \frac{1}{\hbar^2}\sum_{l,r}\left\{(t_{rl})^2\langle a_r^\dagger a_l a_l^\dagger a_r\rangle e^{i(\epsilon_r-\epsilon_l)t/\hbar} + (t_{rl})^2\langle a_l^\dagger a_r a_r^\dagger a_l\rangle e^{-i(\epsilon_r-\epsilon_l)t/\hbar}\right\},\\ &= \frac{1}{\hbar^2}|t|^2\sum_{l,r}\left\{f_R(\epsilon_R)[1-f_L(\epsilon_L)]e^{i(\epsilon_r-\epsilon_l)t/\hbar} + f_L(\epsilon_L)[1-f_R(\epsilon_R)]e^{-i(\epsilon_r-\epsilon_l)t/\hbar}\right\}.\end{aligned} \tag{23}$$

Let us now just take the special case of $\omega \to 0$, i.e. classical noise. Substituting Eq. (23) in Eq. (19) for $\omega = 0$ we have

$$S_{\dot{N}_L}(0) = \frac{2\pi}{\hbar^2}|t|^2\sum_{l,r}\left\{f_R(\epsilon_R)[1-f_L(\epsilon_L)] + f_L(\epsilon_L)[1-f_R(\epsilon_R)]\right\}\delta(\epsilon_r-\epsilon_l). \tag{24}$$

Transforming sum into integral $\sum_{l,r} \to \int d\epsilon_l N_L(\epsilon_l)\int d\epsilon_r N_R(\epsilon_r)$, we have

$$S_{\dot{N}_L}(0) = \frac{2\pi}{\hbar^2}|t|^2 N_L(0)N_R(0)\int d\epsilon\left\{f_R(\epsilon)[1-f_L(\epsilon)] + f_L(\epsilon)[1-f_R(\epsilon)]\right\}. \tag{25}$$

Considering equilibrium, $eV=0$, and $T_L=T_R=T$, Eq. (25) yields

$$\begin{aligned} S_{\dot{N}_L}(0) &= 2\frac{2\pi}{\hbar^2}|t|^2 N_L(0)N_R(0)\int d\epsilon f(\epsilon)[1-f(\epsilon)], \\ &= 2\frac{2\pi}{\hbar^2}|t|^2 N_L(0)N_R(0)k_{\mathrm{B}}T. \end{aligned} \tag{26}$$

The charge current is $I=-e\dot{N}_L$, its noise is then given by

$$\begin{aligned} S_I(0)=e^2 S_{\dot{N}_L}(0) &= 2k_{\mathrm{B}}T\frac{2\pi}{\hbar^2}|t|^2 N_L(0)N_R(0)e^2 \\ &\equiv 2k_{\mathrm{B}}T/R_T, \end{aligned} \tag{27}$$

which is the **Fluctuation-dissipation theorem**.

Problem 7.1: Derive the master equation for $\rho_{ge}$ Eq. (18) in the similar way as for $\rho_{gg}$ in the lecture. (**4 points**)

**The deadline for Problems 7.1 (4 points) is on Tuesday December 1 at noon, before the lecture.**

[1] H.-P. Breuer and F. Petruccione, The theory of open quantum systems (Oxford University Press, New York, 2002).