Recap of lecture 2

previous lecture

$$\dot{\rho} = -i\omega_c' \left[a^\dagger a, \rho\right] + \gamma(\bar{n}+1)\, L[a](\rho) + \gamma \bar{n}\, L[a^\dagger](\rho)$$

↳ $\boxed{\text{Eq 15}}$

where $L[\hat{F}](\rho) \equiv F\rho F^\dagger - \frac{1}{2}\left(F^\dagger F \rho - \rho F^\dagger F\right)$ ↳ $\boxed{\text{Eq 16}}$

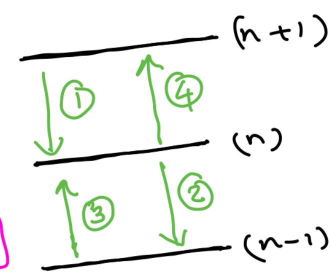
↳ Lindblad Super-operator

(Lindblad Master Equation)

Equations for populations (using above Equation),

$$\dot{P}_n = \overset{1}{\gamma(\bar{n}+1)(n+1)P_{n+1}} - \overset{2}{\gamma(\bar{n}+1)\, n P_n} + \underset{3}{\gamma \bar{n}\, n P_{n-1}} - \underset{4}{\gamma \bar{n}(n+1) P_n}$$

↳ $\boxed{\text{Eq 19}}$



To compute steady state we put $\dot{P}_n = 0$ which gives

$$P_{n+1} = \frac{1}{\gamma(\bar{n}+1)(n+1)}\left[\gamma(\bar{n}+1)\, n P_n + \gamma \bar{n}(n+1) P_n - \gamma \bar{n}\, n P_{n-1}\right]$$

↳ $\boxed{\text{Eq 21}}$

The above Eq. C1 can be solved recursively,

$$P_1 = \left(\frac{\bar{n}}{\bar{n}+1}\right) P_0 \qquad \text{(by putting } n=0\text{)}$$

$$P_2 = \left(\frac{\bar{n}}{\bar{n}+1}\right)^2 P_0 \qquad \text{(by putting } n=1\text{)}$$

$$P_3 = \left(\frac{\bar{n}}{\bar{n}+1}\right)^3 P_0 \qquad \text{(by putting } n=2\text{)}$$

$$\vdots$$

$$P_n = \left(\frac{\bar{n}}{\bar{n}+1}\right)^n P_0$$

The solution of above equations is therefore

$$P_n = \left(\frac{\bar{n}}{n+1}\right)^n P_0 = A^n P_0 \quad \text{where } A = \frac{\bar{n}}{\bar{n}+1} \rightarrow \boxed{Eq\ C2}$$

The constant P_0 is determined by normalization $\sum_{n=0}^{\infty} P_n = 1 \Rightarrow P_0 = 1 - A$

Therefore

$$P_n = A^n (1-A) \rightarrow \boxed{Eq\ C3}$$

$$= \left(\frac{\bar{n}}{\bar{n}+1}\right)^n \frac{1}{(\bar{n}+1)}$$

Remember that $\bar{n} \equiv n(\omega_c, T) = \frac{1}{e^{\omega_c/T} - 1}$

Substituting above equation of $\bar{n}$ into Eq C3 gives

$$P_n = e^{-n\omega_c/T}\left(1 - e^{-\omega_c/T}\right) \rightarrow \boxed{Eq\ C4}$$

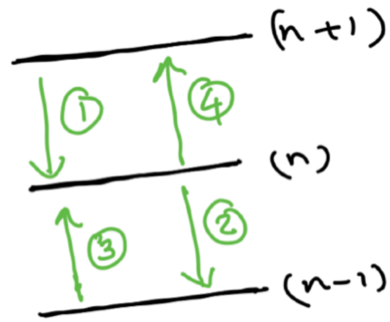
Therefore P_n above agrees with P_n derived from $\rho_{eq} = \frac{e^{-\beta H_s}}{Z}$

Isolated quantum Harmonic oscillator at temperature $T = 1/\beta$

where $Z = \mathrm{Tr}\left(e^{-\beta H_s}\right)$ is the partition function

We can say system acquires the bath-temperature

Detailed balance condition is given by below,



$$\gamma(\bar{n}+1)(n+1)P_{n+1} - \gamma\,\bar{n}(n+1)P_n = 0 \qquad 1 = 4$$

$$\gamma\,\bar{n}\,n\,P_{n-1} - \gamma(\bar{n}+1)\,n\,P_n = 0 \qquad 3 = 2$$

↳ $\boxed{\text{Eq. C5}}$

Note that our steady state solution (which is Eq. C4) satisfies the above detailed balance equation (Eq C5).

We will recap a few things about expectation values of some operator $\hat{O}$

$$\langle \hat{O} \rangle = tr[O\hat{\rho}]$$

$$\langle \dot{a} \rangle = tr[a\dot{\rho}]$$

$$= -i\omega_c' \, tr[aa^\dagger a\rho - a\rho a^\dagger a]$$

$$+ \frac{\gamma}{2} \, tr[2a^2\rho a^\dagger - aa^\dagger a\rho - a\rho a^\dagger a]$$

$$+ \gamma\bar{n} \, tr[a^2\rho a^\dagger + aa^\dagger\rho a - aa^\dagger a\rho - a\rho a a^\dagger]$$

$$= -\left(\frac{\gamma}{2} + i\omega_c'\right) Tr[a\rho]$$

$$= -\left(\frac{\gamma}{2} + i\omega_c'\right)\langle a \rangle \quad \rightarrow \boxed{\text{Eq C6}}$$

For above you need to use cyclic properties of trace and Bosonic commutation $[a, a^\dagger] = 1$.

Similarly for $\langle \hat{n} \rangle = \langle a^\dagger a \rangle$ we have

$$\langle \dot{\hat{n}} \rangle = -\gamma\left(\langle \hat{n} \rangle - \bar{n}\right) \quad - \boxed{\text{Eq C7}}$$

which has solution

$$\langle \hat{n}(t) \rangle = \langle \hat{n}(0) \rangle e^{-\gamma t} + \bar{n}\left(1 - e^{-\gamma t}\right)$$

$$- \boxed{\text{Eq C8}}$$

Therfore

$$\lim_{t\to\infty} \langle \hat{n}(t) \rangle = \bar{n} \quad \text{(steady state)}$$

Lecture-3

Quantum Langevin Equation Method (QLE)

Dhar et al, PRB 73, 085119 (2006)
J Stat phys 125, 801 (2006)

→ Quantum Langevin Equation

→ Comparision between QLE and QME

→ Non-equilibrium transport.

In lecture 1 and 2, we discussed a lot about density matrices. Here, we donot deal with it and instead write full equations of motion (EOM) for system and reservoir.

→ The reservoir degrees of freedom are then eliminated to give Langevin equation for system alone.

→ Finally the Langevin equations are solved by Fourier transforms to obtain steady state properties.

Let us write the Heisenberg EOM (for e.g $\dot{a} = i[H, a]$)

$$\dot{a} = -i\omega_c a - i\sum_j k_j x_j \quad \rightarrow \boxed{Eq. 1}$$

$$\dot{x}_j = -i\omega_j x_j - i k_j^* a \quad \rightarrow \boxed{Eq. 2}$$

There is no restriction on system-bath coupling and there is no Markovian assumption.

One can formally integrate Eq. 2 to get

$$r_j(t) = e^{-i\omega_j(t-t_0)} r_j(t_0) - i K_j^* \int_{t_0}^{\infty} ds\, e^{-i\omega_j(t-s)} \theta(t-s)\, a(s) \quad \rightarrow \boxed{\text{Eq. 3}}$$

By plugging in Eq. 3 into Eq. 1 we get below equation for $\dot{a}(t)$

$$\dot{a}(t) = -i\omega_c a - \int_{t_0}^{\infty} ds\, \Sigma(t-s)\, a(s) + \eta(t) \quad \rightarrow \boxed{\text{Eq. 4}}$$

"Noise" from reservoir

where $\eta(t) = -i \sum_j K_j^* e^{-i\omega_j(t-t_0)} r_j(t_0)$

and $\Sigma(t-s) = \sum_j |K_j|^2 e^{-i\omega_j(t-s)} \theta(t-s) \rightarrow$ "Dissipation" $\rightarrow$ Eq 5

Eq. 4 is the Quantum Langevin Equation. If we are only interested in the steady state we can take $t_0 \to -\infty$. This facilitates going to the Fourier transform.

Our notation for Fourier transform and its inverse are

$$\tilde{F}(\omega) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt\, F(t)\, e^{i\omega t} \quad \text{and} \quad F(t) = \int_{-\infty}^{+\infty} d\omega\, \tilde{F}(\omega)\, e^{-i\omega t} \quad \rightarrow \boxed{\text{Eq 6}}$$

In our case F can represent a, η, Σ. Eq. 4 becomes

$$-i\omega\, \tilde{a}(\omega) + i\omega_c\, \tilde{a}(\omega) - 2\pi\, \tilde{\Sigma}(\omega)\, \tilde{a}(\omega) = \tilde{\eta}(\omega) \quad \rightarrow \boxed{\text{Eq 7}}$$

which yields

$$\tilde{a}(\omega) = \frac{\tilde{\eta}(\omega)}{i(\omega_c - \omega) - 2\pi\tilde{\Sigma}(\omega)} \quad \rightarrow \boxed{\text{Eq. 8}}$$

Let us compute the steady state (ss) value of the bosonic occupation number $\langle \hat{n}(t) \rangle$

$$\langle a^{\dagger}(t) a(t) \rangle_{ss} = \int_{-\infty}^{+\infty} d\omega\, d\omega'\, e^{i(\omega-\omega')t} \langle \hat{a}^{\dagger}(\omega) \hat{a}(\omega') \rangle$$

$$= \int_{-\infty}^{+\infty} d\omega\, d\omega' \frac{e^{i(\omega-\omega')t} \langle \hat{\eta}^{\dagger}(\omega) \hat{\eta}(\omega') \rangle}{\left[i(\omega_c-\omega) - 2\pi \Sigma(\omega)\right]\left[-i(\omega_c-\omega') - 2\pi \Sigma^{*}(\omega')\right]}$$

$\hookrightarrow \boxed{\text{Eq. 9}}$

It is clear from Eq. 9 that we need $\langle \hat{\eta}^{\dagger}(\omega) \hat{\eta}(\omega') \rangle$ and $\Sigma(\omega)$. Let us choose the reservoir to be at temperature T. Using Eq. 5 and after some algebra, we get

$$\langle \hat{\eta}^{\dagger}(\omega) \hat{\eta}(\omega') \rangle = \frac{\alpha(\omega)}{\pi} \bar{n}(\omega) \delta(\omega-\omega')$$

$$\tilde{\Sigma}(\omega) = \frac{1}{2\pi} \alpha(\omega) - \frac{i}{2\pi} \Delta(\omega)$$

$\rightarrow \boxed{\text{Eq. 10.}}$

where recall that $\bar{n}(\omega) = \dfrac{1}{e^{\omega/k_B T} - 1}$

Note that $\alpha(\omega)$, $\Delta(\omega)$ in Eq. 10 are given by

$$\alpha(\omega) = \pi g(\omega) |K(\omega)|^2$$

$$\Delta(\omega) = P \int_{0}^{\infty} d\bar{\omega} \frac{g(\bar{\omega}) |K(\bar{\omega})|^2}{\bar{\omega} - \omega}$$

$\rightarrow \boxed{\text{Eq. 11}}$

Hence we get

$$\langle \hat{n}(t) \rangle_{ss}^{QLE} = \langle a^{\dagger}(t) a(t) \rangle_{ss}^{QLE} = \frac{1}{\pi} \int_{-\infty}^{+\infty} d\omega \left[\frac{\alpha(\omega) \bar{n}(\omega)}{(\omega - \omega_c - \Delta(\omega))^2 + (\alpha(\omega))^2} \right]$$

$\hookrightarrow \boxed{\text{Eq. 12}}$

Eq 12 is exact result from QLE valid for any System-bath coupling. The system-bath coupling information is encoded in $\alpha(\omega)$ and $\Delta(\omega)$.

One knows from QME (previous lecture) that

$$\langle \hat{n}(t) \rangle_{ss}^{QME} = \bar{n}(\omega_c) \quad \rightarrow \boxed{\text{Eq 13}}$$

If we take the careful limit of system-bath coupling to zero we get

$$\lim_{\substack{\text{system} \\ \text{-Bath}} \to 0} \langle \hat{n}(t) \rangle_{ss}^{QLE} = \langle \hat{n}(t) \rangle_{ss}^{QME} = \bar{n}(\omega_c) \quad \rightarrow \boxed{\text{Eq 14}}$$

It is to be noted that taking weak system-bath coupling limit is a subtle issue. This limit basically results in the appearance of a Dirac delta function in Eq. 12 which picks up $\bar{n}(\omega_c)$.

Using QLE one can also compute two-time averages,

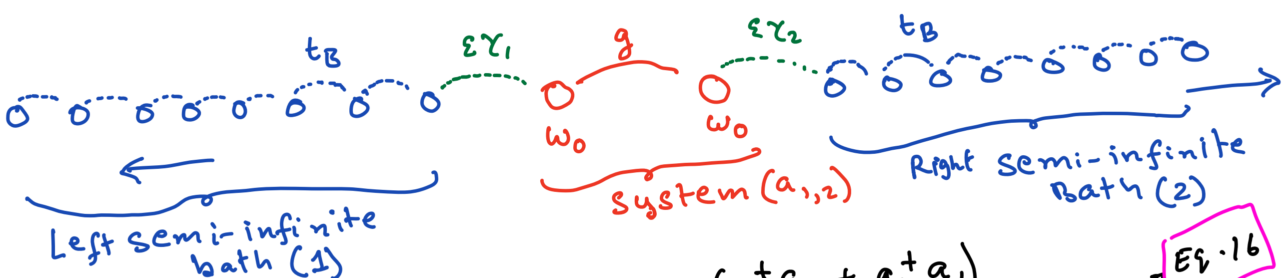
$$\lim_{t \to \infty} \langle a^{+}(t) a(t+\tau) \rangle = \frac{1}{\pi} \int_{-\infty}^{+\infty} d\omega \, \frac{\alpha(\omega)\, \bar{n}(\omega)\, e^{-i\omega\tau}}{[\omega - \omega_0 - \Delta(\omega)]^2 + [\alpha(\omega)]^2} \quad \rightarrow \boxed{\text{Eq. 15}}$$

Similarly one can compute multi-point correlation functions using QLE. Such correlation functions are very relavant in experiments also

Computing non-equilibrium steady state current using QLE

[Purkayastha, Dhar, Kulkarni, PRA 93, 062114 (2016)]

Let us consider a situation where a system is coupled to two reservoirs. In particular we consider a two-site system coupled to baths with are semi-infinite one-dimensional chains



$$H_S = w_0(a_1^\dagger a_1 + a_2^\dagger a_2) + g(a_1^\dagger a_2 + a_2^\dagger a_1) \quad \rightarrow \boxed{\text{Eq.16}}$$

Bath index

$$H_B^{(l)} = t_B\left(\sum_{s=1}^{\infty} b_s^{(l)\dagger} b_{s+1}^{(l)} + h.c.\right), \quad \hat{H}_B = \underbrace{\hat{H}_B^{(1)}}_{\text{left Bath}} + \underbrace{\hat{H}_B^{(2)}}_{\text{right bath}}$$

$$H_{SB} = \underbrace{\varepsilon\gamma_1\left(a_1^\dagger b_1^{(1)} + h.c.\right)}_{\text{left system-bath coupling}} + \underbrace{\varepsilon\gamma_2\left(a_2^\dagger b_1^{(2)} + H.c.\right)}_{\text{right system-bath coupling}}$$

Let us discuss how to approach the above problem with QLE.

(i) First, go to eigenmodes of the bath

$$H_B^{(l)} = t_B\left(\sum_{s=1}^{\infty} b_s^{(l)\dagger} b_{s+1}^{(l)} + H.c.\right) = \sum_{r=1}^{\infty} \Omega_r^{(l)} B_r^{(l)\dagger} B_r^{(l)} \quad \rightarrow \boxed{\text{Eq 17}}$$

Here $b_s^{(l)} = \sum_r U_{rs}^{l*} B_r^l$ where U is a unitary matrix that diagonalizes $\hat{H}_B^{(l)}$.

$B_r^{(\ell)}$ is the anhillation operator of the eigenmode with eigenvalue Ω_r^{ℓ}. The bath eigen-modes satisfy the initial bath correlation functions: $\langle \hat{B}_r^{\ell} \rangle = 0$ and $\langle B_r^{(\ell)\dagger} B_s^{(\ell)} \rangle = n_\ell(\Omega_r^{(\ell)})\, \delta_{rs}$.

We also have $K_{\ell r} = \tau_\ell U_{r1}^{(\ell)*}$. The EOM for system and bath are

$$\frac{dB_r^{(\ell)}}{dt} = -i\left(\Omega_r^{(\ell)} B_r^{(\ell)} + \varepsilon K_{\ell r}^{*} a_\ell\right)$$

$$\frac{da_1}{dt} = -i\left(\omega_0 a_1 + g a_2 + \sum_r \varepsilon K_{1r} B_r^{(1)}\right)$$

same for a_2 with $1 \Longleftrightarrow 2$

$\hookrightarrow$ Eq. 18

We can adapt the same procedure as described in the earlier part of the lecture and we get,

current in the 1-2 Bond

$$I_{1\to 2} = -ig\langle a_1^\dagger a_2 - a_2^\dagger a_1\rangle = g^2\varepsilon^2 \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{J_1(\omega) J_2(\omega)\left(n_1(\omega) - n_2(\omega)\right)}{|M(\omega)|^2}$$

$$\langle a_1^\dagger a_1\rangle = \varepsilon \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi}\left[\frac{K(\omega) J_1(\omega)\, n_1(\omega)}{|M(\omega)|^2} + \frac{g^2 J_2(\omega) n_2(\omega)}{|M(\omega)|^2}\right]$$

$\hookrightarrow$ Eq. 19

where some definitions are given below.

$$\Delta_\ell(\omega) = P\int_{-\infty}^{+\infty} \frac{d\omega'}{2\pi} \frac{J_\ell(\omega')}{\omega - \omega'}$$

$$M(\omega) = \left[\left(\omega_0 - \omega - i\varepsilon^2 \frac{J_1(\omega)}{2} + \varepsilon^2 \Delta_1(\omega)\right)\left(\omega_0 - \omega - i\varepsilon^2 \frac{J_2(\omega)}{2} + \varepsilon^2 \Delta_2(\omega)\right) - g^2\right]$$

$$K(\omega) = \left|\omega_0 - \omega - i\varepsilon^2 \frac{J_2(\omega)}{2} + \varepsilon^2 \Delta_2(\omega)\right|^2$$

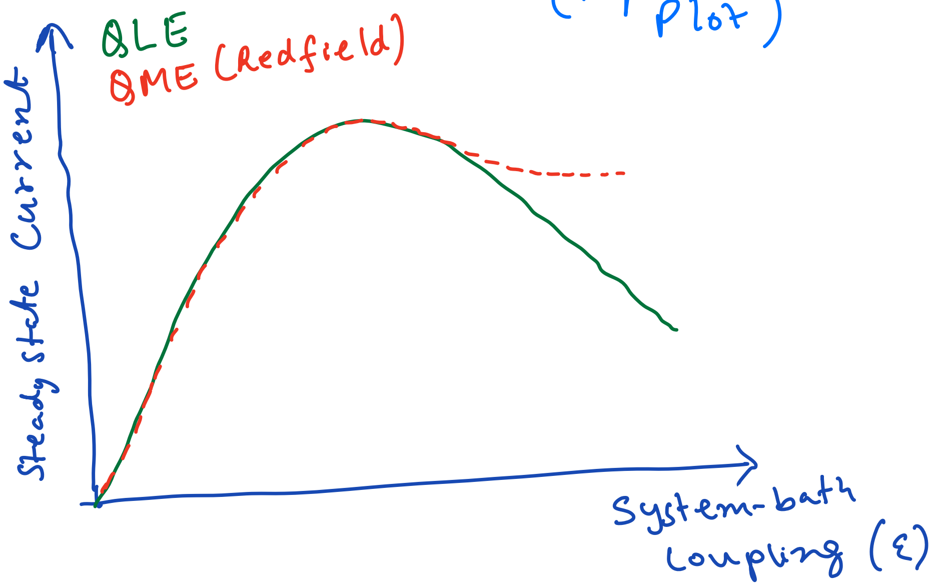
$\hookrightarrow$ Eq. 20

Note that the bath spectral function in summation form is $J_\ell(\omega) = 2\pi \sum_r |K_{\ell r}|^2 \, \delta(\omega - \Omega_r^\ell)$

In above case, this can be explicitly computed to give
$$J_\ell(\omega) = \frac{2\gamma_\ell^2}{t_B} \sqrt{1 - \left(\frac{\omega}{2t_B}\right)^2} . \quad \rightarrow \boxed{\text{Eq. 21}}$$

Note that Eq 19 for currents and bosonic occupation number is exact for any value of system bath coupling. In other words if we had done a Born-Markov approximation (Redfield) for Eq. 16, the results would start deviating for large ε.

(Representative plot)



Exact Numerical Results for Eq. 16 (Time dynamics)

→ To check time dynamics one can do numerical simulations by choosing bath to be of finite (but large say 511 each) size and evolving full system-bath Hamiltonian $\hat{H}$ using unitary Hamiltonian dynamics.

→ Collectively denote by "d" a coloumn vector with all anhillation operators of both system and bath.

→ The full hamiltonian can be written as $\hat{H} = \sum_{ij} H_{ij} d_i^{+} d_j$ where "i" stands for either system or bath sites.

Eq. 22

→ If $D = \langle d\, d^{+} \rangle$ denotes full correlation matrix of system + bath then its time evolution is given by $D(t) = e^{iHt} D\, e^{-iHt}$

Matrix equation for correlations.

Temperatures / chemical potentials of the bath enter here.

Summary Table: Harmonic Oscillator coupled to Baths (and various generalizations)

	System-Bath coupling	Time Dynamics	Multi-point correlations
Quantum Master Equation	Perturbative	Possible	Possible using Quantum Regression Theorem
Quantum Langevin Equation	Non-perturbative	Very difficult (almost impossible)	Possible (but steady state)
Direct numerics (large but finite number of reservoirs)	Non-perturbative	Possible	Possible

In the next lecture, we will talk about open two-level /multi-level systems.