Statistical mixtures in quantum mech. (1)

System + environment always in pure state (assume)

$$|\Psi\rangle = \sum_{jk} c_{jk} |\varphi_j\rangle \otimes |\eta_k\rangle$$

This implies no description in terms of a "pure" quantum state of the system.
What is important in q.m is measurement
If O_s observable of the system, what is the exp. val. on $|\Psi\rangle$?

$$\langle O_s\rangle = \langle\Psi| O_s \otimes \mathbb{I}_E |\Psi\rangle$$

$$= \sum_{\substack{jk\\ em}} c^*_{em} c_{jk} \langle\varphi_e|O_s|\varphi_j\rangle \underbrace{\langle\eta_m|\eta_k\rangle}_{\delta_{km}}$$

$$= \sum_{je} \sum_{m} c^*_{em} c_{jm} \langle\varphi_e|O_s|\varphi_j\rangle$$

$$= \sum_{je} \rho_{je} O_{s_{ej}} = \mathrm{Tr}(\rho O_s)$$

$$\rho_{je} = \sum_m c^*_{em} c_{jm}$$

$$= \sum_m \langle\varphi_e| \otimes \langle\eta_m|\Psi\rangle\langle\Psi|\eta_m\rangle \otimes |\varphi_j\rangle$$

$$\hat{\rho} = \sum_m |\varphi_e\rangle \langle \varphi_e \eta_m | \Psi \rangle \langle \Psi | \varphi_j \eta_m \rangle \langle \varphi_j |$$

$$= \mathrm{Tr}_B \left(|\Psi\rangle\langle\Psi| \right) \quad \text{partial trace}$$

$\hat{\rho}$ operator : $\mathcal{H}_s \to \mathcal{H}_s$

1. $\hat{\rho}^+ = \hat{\rho}$
2. $\mathrm{Tr}(\hat{\rho}) = \sum_{jm} |c_{jm}|^2 = 1$
3. $\langle \varphi | \hat{\rho} | \varphi \rangle \geq 0 \quad \forall |\varphi\rangle \in \mathcal{H}_s$

Spectral decomp.

$$\hat{\rho} = \sum_j p_j |\varphi_j\rangle\langle\varphi_j| \qquad \sum_j p_j = 1 \quad 1 \geq p_j \geq 0$$

not unique if $|\varphi_j\rangle$ not orthogonal.

$$\mathrm{Tr}(\hat{\rho}^2) \leq \mathrm{Tr}(\hat{\rho}) = 1$$

If we have a pure state $|\Psi\rangle$ and an obs. O, then

$\langle O \rangle = \langle \Psi | O | \Psi \rangle = \mathrm{Tr}(O |\Psi\rangle\langle\Psi|)$

Then, for a quantum state ("pure")

$\hat{\rho} = |\Psi\rangle\langle\Psi|$

$\mathrm{Tr}(\hat{\rho}^2) = 1$ pure state ... cond.

Define $S(\mathcal{H}_s)$ Liouville space of D.M.

If $\rho_1, \rho_2 \in S(\mathcal{H}_s) \Rightarrow$

$\rho = \lambda \rho_1 + (1-\lambda)\rho_2 \in S(\mathcal{H}_s) \quad \lambda \in [0,1]$

~~convex~~. property of $S(\mathcal{H}_s)$

pure states live at the boundary of $S(\mathcal{H}_s)$ and cannot be expressed as convex linear comb. of nontrivial d.m.'s.

The adv. of the d.m. formalism is that of unifying statistical mixtures and pure states.

$$\rho = \sum_j p_j |\varphi_j\rangle\langle\varphi_j|$$

$$\langle O \rangle = \mathrm{Tr}(O\rho) = \sum_j p_j \langle\varphi_j|O|\varphi_j\rangle$$

$$= \sum_j p_j \langle O \rangle_j$$

from which the notion of stat. mixture becomes clear.

If two subsystems are not correlated, then

$$\rho = \rho_1 \otimes \rho_2$$

this means. $\hat{A} = \hat{A}_1 \otimes \hat{A}_2$

$$\langle \hat{A} \rangle = \mathrm{Tr}(\hat{A}\hat{\rho}) =$$

$$= \mathrm{Tr}_1(A_1\rho_1)\,\mathrm{Tr}_2(A_2\rho_2)$$

$$= \langle A_1 \rangle \langle A_2 \rangle$$

However in general, if $\rho_j = \mathrm{Tr}_{s/j}(\rho)$

it is not true that

$$\rho = \rho_1 \otimes \rho_2$$

because there can be entanglement.

Notion of separability for DM

As the whole q. m. can be formulated in terms of density m., we derive now the time evolution equation for the d. m.

Closed quantum system.

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle$$

$$|\psi(t)\rangle = U(t,0) |\psi(0)\rangle$$

$$i \frac{\partial}{\partial t} U(t,0) = H(t) U(t,0) \qquad U(0,0) = \mathbb{I}$$

If $H(t) = H \Rightarrow U(t,0) = e^{-iHt/\hbar}$

otherwise
$$U(t,0) = T \exp\left[-i \int_{t_0}^{t} ds \, H(s)\right]$$

If at $t=0$ $\quad \rho = \sum_j p_j |\varphi_j\rangle\langle\varphi_j|$

$$\Rightarrow \rho(t) = \sum_j p_j \, U(t,0) |\varphi_j\rangle \langle\varphi_j| U^+(t,0)$$
$$= U(t,0) \rho(0) U^+(t,0)$$

$$\Rightarrow \boxed{\frac{d}{dt} \rho(t) = -i [H(t), \rho(t)]}$$

Liouville - Von Neumann equation

$$\frac{d\rho(t)}{dt} = \mathcal{L}(t)\rho(t)$$

$\mathcal{L}(t)$ Liouville super-operator

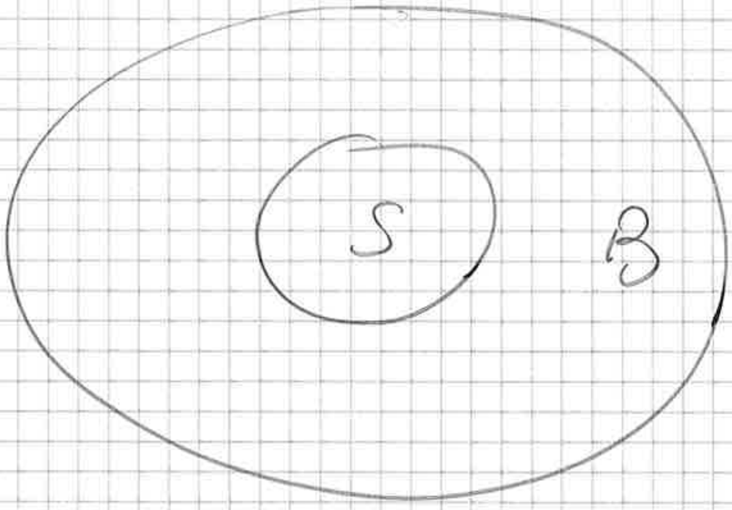
$$\rho(t) = T \exp\left[\int_{t_0}^{t} ds\, \mathcal{L}(s)\right] \rho(t_0)$$

For $\mathcal{L}(t) = \mathcal{L}$

$$\rho(t) = \exp(\mathcal{L}t)\,\rho(0)$$

We now wish to describe an open Q. S. S coupled to another system B the <u>environment</u> (naming)

Total Hilbert space $\mathcal{H}_S \otimes \mathcal{H}_B$



$$H = H_S \otimes I_B + I_S \otimes H_B + H_I(t)$$

Why do so?

- $S + B$ too big to be modeled
- interested only in observables of S
- B not well known.

Observables of S : $A \otimes I_B$

$\langle A \rangle = Tr_S(A\rho_S)$ partial trace

$\rho_S = Tr_B(\rho)$

<u>Interest in knowing</u> $\underline{\rho_S(t)}$

$$\rho_S(t) = \mathrm{Tr}_B(\rho(t))$$
$$= \mathrm{Tr}_B\left(U(t,t_0)\,\rho(t_0)\,U^{+}(t,t_0)\right)$$

If S + B form a closed system, then

$$\frac{d\rho_S(t)}{dt} = -i\,\mathrm{Tr}_B\left(\left[H(t), \rho(t)\right]\right)$$

Quantum Markovian process

A Markovian environment is one for which the timescale associated to the correlations is much shorter than any timescale relevant to the system dynamics. This condition implies the absence of any memory effect for the reduced system dynamics.

A more formal definition of a quantum Markov process can be introduced in relation to the dynamical map.

At $t=0$ the full density matrix is assumed to be the uncorrelated system-environment state

$$\rho(0) = \rho_S(0) \otimes \rho_B$$

The time evolution is then

$$\rho_S(0) \longrightarrow \rho_S(t) = \mathrm{Tr}_B\left(\hat{U}(t,0)\left[\rho_S(0)\otimes\rho_B\right]\hat{U}^{+}(t,0)\right)$$

$$\equiv V(t)\,\rho_S(0)$$

Here $V(t): S \longrightarrow S$ is a map from the space of reduced density matrices into itself. called the <u>dynamical map</u>

Then as a function of time t we have a family of maps $\{V(t) \mid t \geq 0\}$ with $V(0) = \text{identity}$.

The Markovian property is then translated into the semigroup property (in the homogeneous case)

$$V(t_1)V(t_2) = V(t_1 + t_2) \qquad t_1, t_2 \geq 0$$

In other words, if $\rho_s(t_2) = V(t_2)\rho_s(0)$, then at $t = t_1 + t_2$ the state $\rho_s(t_1 + t_2)$ will only depend on $\rho_s(t_2)$ and not on its past history.

The quantum dynamical semigroup property is analogous to the Chapman-Kolmogorov equation holding for classical stochastic processes. Its homogeneous version is

$$P_{\tau+\tau'}(x \mid x') = \int dx'' \, P_\tau(x \mid x'') \, P_{\tau'}(x'' \mid x')$$

$$\tau, \tau' \geq 0$$

which has an intuitive interpretation.

Under general conditions,* it is possible to write a quantum dynamical semigroup in terms of a generator $\mathcal{L}$ as

$$V(t) = \exp(\mathcal{L} t)$$

which implies the differential equation

$$\frac{d}{dt} \rho_s(t) = \mathcal{L} \rho_s(t)$$

which is called the Markovian quantum master equation.

The generator $\mathcal{L}$ is a linear super-operator $\mathcal{L} : S \to S$ called Liouvillian.

For the case of an isolated system we have seen that

$$\mathcal{L} \rho(t) = -i [H, \rho(t)]$$

Highlight that this is a Markov process as the schr. eq. can be solved from the initial condition only

* Bounded $\mathcal{L}$, separable (Metric) $\mathcal{H}_S$

For most physical systems $\mathcal{L}$ is not bound (neither is H).

We now wish to determine the form of $V(t)$ and of the Liouvillian $\mathcal{L}$ from general principles, retaining only the Markov assumption.

We introduce the spectral decomposition of the bath density matrix

$$\rho_B = \sum_\alpha \lambda_\alpha |\varphi_\alpha\rangle\langle\varphi_\alpha| \qquad \sum_\alpha \lambda_\alpha = 1 \quad \lambda_\alpha \geq 0$$

Then $$V(t)\rho_s = \mathrm{tr}_B\left(U(t,0)\, \rho_s \otimes \rho_B\, U^+(t,0)\right)$$

$$= \sum_\alpha \langle\varphi_\alpha| U(t,0)\, \rho_s \otimes \rho_B\, U^+(t,0) |\varphi_\alpha\rangle$$

$$= \sum_{\alpha,\beta} \sqrt{\lambda_\beta}\, \langle\varphi_\alpha|U(t,0)|\varphi_\beta\rangle\, \rho_s\, \langle\varphi_\beta|U^+(t,0)|\varphi_\alpha\rangle \sqrt{\lambda_\beta}$$

$$= \sum_{\alpha,\beta} W_{\alpha\beta}(t)\, \rho_s\, W^+_{\alpha\beta}(t)$$

$$W_{\alpha\beta}(t) : \mathcal{H}_s \to \mathcal{H}_s$$

$$W_{\alpha\beta}(t) = \sqrt{\lambda_\beta}\, \langle\varphi_\alpha| U(t,0) |\varphi_\beta\rangle$$

(Pay attention to the fact that U is an operator on $\mathcal{H}_s \otimes \mathcal{H}_B$ and that taking matrix elements over bath states $|\varphi_\alpha\rangle$ results into an operator $W : \mathcal{H}_s \to \mathcal{H}_s$)

We see that $\sum_{\alpha\beta} W^+_{\alpha\beta}(t)\, W_{\alpha\beta}(t) = \mathbb{1}$

Then $$\mathrm{Tr}_s\left(V(t)\rho_s\right) = \sum_{\alpha\beta} \mathrm{Tr}_s\left(W_{\alpha\beta}\, \rho_s\, W^+_{\alpha\beta}\right)$$

$$= \mathrm{Tr}_s\left(\sum_{\alpha\beta} W^+_{\alpha\beta} W_{\alpha\beta}\, \rho_s\right)$$

$$= \mathrm{Tr}_S(\rho_S) = 1$$

Thus $V(t)$ is a linear, trace preserving map. It is also completely positive:

$$\langle \varphi | \sum_{\alpha\beta} W_{\alpha\beta}\, \rho_S\, W^{\dagger}_{\alpha\beta} | \varphi \rangle =$$

$$= \sum_{\alpha\beta} \langle \varphi_{\alpha\beta} | \rho_S | \varphi_{\alpha\beta} \rangle \geq 0$$ from the positivity of ρ_S

To derive the general form of $\mathcal{L}$, we assume a finite dimensional Hilbert space for the system, $\mathcal{H}_S$, with dimension N. The present considerations can be extended to infinite dimension in the case of countable states, assuming $\mathcal{L}$ is bounded. More generally, a different strategy is adopted, namely to derive $\mathcal{L}$ microscopically for a specific model, and realize that it has the general form that we are going to derive below.

Consider the N^2-dimensional space of operators on $\mathcal{H}_S$. Consider a set of orthonormal operators $\hat{F}_j$, $j = 1, 2, \ldots, N^2$ such that

$$\left(\hat{F}_j, \hat{F}_k\right) = \mathrm{Tr}_S\left(\hat{F}_j^\dagger \hat{F}_k\right) = \delta_{jk}$$

(this scalar product is the one defining the trace distance).

One of the F_j is assumed proportional to $\mathbb{I}_S$

$\hat{F}_{N^2} = \frac{1}{\sqrt{N}} \mathbb{I}_S$. Then all other F's are traceless,

$\mathrm{Tr}_S\left(F_j\right) = 0 \quad j = 1, \ldots, N^2-1$

Let us expand each $W_{\alpha\beta}$ on this basis

$$\hat{W}_{\alpha\beta}(t) = \sum_{j=1}^{N^2} \hat{F}_j \left(\hat{F}_j, \hat{W}_{\alpha\beta}\right)$$

Then

$$V(t)\,\rho_S = \sum_{j,k=1}^{N^2} c_{jk}(t)\, \hat{F}_j\, \rho_S\, \hat{F}_k^\dagger$$

$$c_{jk}(t) = \sum_{\alpha\beta} \left(F_j, W_{\alpha\beta}(t)\right)\left(F_k, W_{\alpha\beta}(t)\right)^*$$

The matrix c_{jk} is hermitian and positive by construction.

We can now write $\mathcal{L}\rho_s$ as:

$$\mathcal{L}\rho_s = \lim_{\varepsilon\to 0} \frac{1}{\varepsilon}\left(V(\varepsilon)\rho_s - \rho_s\right)$$

By defining a_{jk} as (a_{jk} is hermitian and positive)

$$a_{N^2N^2} = \lim_{\varepsilon\to 0} \frac{c_{N^2N^2}(\varepsilon) - N}{\varepsilon}$$

$$a_{jN^2} = \lim_{\varepsilon\to 0} \frac{c_{jN^2}(\varepsilon)}{\varepsilon}$$

$$a_{jk} = \lim_{\varepsilon\to 0} \frac{c_{jk}(\varepsilon)}{\varepsilon}$$

$$\hat{F} = \frac{1}{\sqrt{N}} \sum_{j=1}^{N^2-1} a_{jN^2} \hat{F}_j$$

$$\hat{G} = \frac{1}{2N} a_{N^2N^2} \hat{\mathbb{I}}_s + \frac{1}{2}\left(\hat{F}^{+} + \hat{F}\right)$$

$$\hat{H} = \frac{1}{2i}\left(\hat{F}^{+} - \hat{F}\right)$$

we have

$$\mathcal{L}\rho_s = -i\left[H, \rho_s\right] + \left\{G, \rho_s\right\} + \sum_{j,k=1}^{N^2-1} a_{jk} \hat{F}_j \rho_s \hat{F}_k^{+}$$

From $Tr_s(\mathcal{L}\rho_s) = 0 \ \forall \rho_s$ we have

$$G = -\frac{1}{2} \sum_{j,k=1}^{N^2-1} a_{jk} \hat{F}_j^{+} \hat{F}_k$$

then

$$\boxed{\mathcal{L}\rho_s = -i\left[H, \rho_s\right] + \sum_{j,k=1}^{N^2-1} a_{jk}\left(\hat{F}_j \rho_s F_k^{+} - \frac{1}{2}\left\{F_j^{+} F_k, \rho_s\right\}\right)}$$

Since a_{jk} is positive and Hermitian, it can be diagonalized by a unitary transf.

$$\hat{u}: \quad u a u^{+} = \begin{pmatrix} \gamma_1 & & 0 \\ & \ddots & \\ 0 & & \gamma_{N^2-1} \end{pmatrix} \qquad \gamma_j \geq 0$$

Define then $\hat{F}_j = \sum_{k=1}^{N^2-1} u_{kj} \hat{A}_k$

one can finally express the Liouvillian in diagonal form as

$$\boxed{\mathcal{L}\rho_S = -i\left[H, \rho_S\right] + \sum_{k=1}^{N^2-1} \gamma_k \left(A_k \rho_S A_k^{+} - \frac{1}{2} A_k^{+} A_k \rho_S - \frac{1}{2} \rho_S A_k^{+} A_k\right)}$$

which is the most general form of the generator of a quantum dynamical semigroup.

A_k : Lindblad operators

γ_k : (inverse time) relaxation rates, linked to correlation functions of the environment

Dissipator: $\mathcal{D}(\rho_S) = \sum_k \gamma_k \left(A_k \rho_S A_k^{+} - \frac{1}{2} A_k^{+} A_k \rho_S - \frac{1}{2} \rho_S A_k^{+} A_k\right)$

$$\boxed{\frac{d \rho_S(t)}{dt} = -i\left[H, \rho_S(t)\right] + \mathcal{D}(\rho_S(t))}$$

Operators H and A_n are not linked to Hamiltonian and local system op. in general.

They are also not unique. $\mathcal{L}$ is invariant under the transformations:

1. Unitary transf of A_k

$$\sqrt{\gamma_k}\, A_k \to \sqrt{\gamma_k'}\, A_k' = \sum_j u_{kj} \sqrt{\gamma_j}\, A_j$$

2. Inhomog. transf.

$$A_k \to A_k' = A_k + a_k$$

$$H \to H' = H + \frac{1}{2i} \sum_j \gamma_j \left(a_j^* A_j - a_j A_j^+ \right) + b$$

$$a_k \in \mathbb{C} \qquad b \in \mathbb{R}$$

Also possible to have time-dep. generator

$$\frac{d}{dt} \rho_s(t) = \mathcal{L}(t) \rho_s(t)$$

then $\quad V(t, t_0) = T \exp\left(\int_{t_0}^{t} ds\, \mathcal{L}(s) \right)$

$$\frac{\partial V(t, t_0)}{\partial t} = \mathcal{L}(t) V(t, t_0)$$

$$V(t, t_0) = V(t, t_1) V(t_1, t_0)$$

How to derive H and A_n explicitly.
Possible within given approximation schemes.

1 Weak coupling limit

Interaction between S and B is weak so that ρ_B is approximately not affected by the system.

- Introduce 2nd order Born approx

$$\rho(t) \simeq \rho_S(t) \otimes \rho_B$$

true only on a coarse-grained time:
S affects B but B decays very rapidly back to ρ_B

- Introduce Markov approximation

$$\rho_S(s) \text{ retarded time} \simeq \rho_S(t)$$

Togethere, they for the Born-Markov. approx
Condition: bath correl. time $\boxed{\tau_B \ll \tau_R}$
τ_R rel time of the system, over which the state of S varies appreciably

- Secular or rotating-wave approx. Requires $\boxed{\tau_S \simeq |\omega-\omega'|^{-1} \ll \tau_R}$

In this limit therefore, we need both the internal system dynamics and the Bath dynamics to be much faster than the relax time T_R induced by the Bath onto the system

Then:

$$\frac{d\rho_s(t)}{dt} = -i\left[H + H_{LS}, \rho_s(t)\right] + D(\rho_s(t))$$

$$H_{LS} = \sum_{\omega} \sum_{\alpha,\beta} S_{\alpha\beta}(\omega) A^{+}_{\alpha}(\omega) A_{\beta}(\omega)$$

Lamb-shift Hamiltonian

$$D(\rho_s) = \sum_{\omega} \sum_{\alpha\beta} \gamma_{\alpha\beta}(\omega)\left(A_{\beta}(\omega)\rho_s A^{+}_{\alpha}(\omega) - \frac{1}{2}\left\{A^{+}_{\alpha}(\omega)A_{\beta}(\omega), \rho_s(t)\right\}\right)$$

where $\Gamma_{\alpha\beta}(\omega) = \frac{1}{2}\gamma_{\alpha\beta}(\omega) + i S_{\alpha\beta}(\omega)$

are correl. functions of the reservoir

$$\Gamma_{\alpha\beta}(\omega) = \int_0^{\infty} ds\, e^{i\omega s} \left\langle B^{+}_{\alpha}(s) B_{\alpha}(0)\right\rangle$$

$$H_I = \sum_{\alpha} \hat{A}_{\alpha} \otimes \hat{B}_{\alpha}$$

$$\boxed{A_{\alpha}(\omega) = \sum_{\varepsilon'-\varepsilon=\omega} \Pi(\varepsilon) A_{\alpha} \Pi(\varepsilon')}$$

Very important. Environment induces transitions through system eigenstates

$\Pi(\varepsilon)$ is the projector on the ~~de~~ eigenstate system subspace at energy ε.

<u>In particular</u>

$$[H_S, A_\alpha(\omega)] = -\omega A_\alpha(\omega)$$

$$[H_S, A_\alpha^+(\omega)] = +\omega A_\alpha^+(\omega)$$

In most treatments of open many-body QS, this is neglected. and local (i.e. non-interacting) operators are used instead.

<u>Example</u> : 1 cavity mode

$H_S = \hbar\omega a^+ a$

then $\hat{a}$ and $\hat{a}^+$ are eigenoperators

then $\dot{\rho}_S = -i[H_S, \rho_S] + \gamma\left(a\rho_S a^+ - \frac{1}{2}a^+ a\rho_S - \frac{1}{2}\rho_S a^+ a\right)$

This is correct. However two coupled cavity modes

$H_S = \hbar\omega_1 a_1^+ a_1 + \hbar\omega_2 a_2^+ a_2 + J(a_1^+ a_2 + a_2^+ a_1)$

we will always see

$$D(\rho_s) = \sum_{j=1,2} \gamma_j \left(a_j \rho_s a_j^+ - \frac{1}{2} a_j^+ a_j \rho_s - \frac{1}{2} \rho_s a_j^+ a_j \right)$$

but this is not in line with what seen previously because eigen-operators are $\tilde{a}_j = U_{jk} \hat{a}_k$ (because of the coupling)

Ideally, solving a model of an open quantum system requires to diagonalize the system Hamiltonian first.

Example: Quantum optical master eq.

$$H_B = \sum_{\vec{k}} \sum_{\lambda=1,2} \hbar \omega_k b_\lambda^\dagger(\vec{k}) b_\lambda(\vec{k})$$

Electrom. field

$$\vec{E} = i \sum_{k} \sum_{\lambda=1,2} \sqrt{\frac{2\pi\hbar\omega_k}{V}} \vec{\varepsilon}_\lambda(\vec{k}) \left(b_\lambda(\vec{k}) - b_\lambda^\dagger(k) \right)$$

$$\hat{H}_I = -\vec{D} \cdot \vec{E}$$ $\vec{D}$ dipole op. of the system

$$\vec{A}(\omega) = \sum_{\varepsilon' - \varepsilon = \omega} \Pi(\varepsilon) \vec{D} \Pi(\varepsilon')$$

$$\vec{D}(t) = \sum_{\omega} e^{-i\omega t} \vec{A}(\omega)$$

Assuming a thermal bath

$$\rho_B = \frac{1}{Z_B} e^{-\beta H_B} \qquad \beta = \frac{1}{k_B T}$$

$$\langle b_\lambda^\dagger(k) b_{\lambda'}(k') \rangle = \delta_{kk'} \delta_{\lambda\lambda'} N(\omega_k)$$

$$\langle b_\lambda(k) b_{\lambda'}^\dagger(k') \rangle = \delta \; \delta \quad 1 + N(\omega_k)$$

$$N(\omega) = \frac{1}{e^{\beta\omega} - 1}$$

one finally gets

$$\frac{d\rho_s}{dt} = -\frac{i}{\hbar}\left[H + H_{LS}, \rho_s\right] + \mathcal{D}(\rho_s)$$

$$H_{LS} = \sum_{\omega} \hbar S(\omega)\, \vec{A}^{+}(\omega) \cdot \vec{A}(\omega)$$

$$\mathcal{D}(\rho_s) = \sum_{\omega > 0} \frac{4\omega^3}{3\hbar c^3}\left(1 + N(\omega)\right)\left(\vec{A}(\omega)\rho_s \vec{A}^{+}(\omega) - \frac{1}{2}\left\{\vec{A}^{+}(\omega)\cdot\vec{A}(\omega), \rho_s\right\}\right)$$

$$+ \sum_{\omega > 0} \frac{4\omega^3}{3\hbar c^3} N(\omega)\left(\vec{A}^{+}(\omega)\rho_s \vec{A}(\omega) - \frac{1}{2}\left\{\vec{A}(\omega)\cdot\vec{A}^{+}(\omega), \rho_s\right\}\right)$$

$S(\omega)$: structure factor

$$= \frac{2}{3\pi\hbar c^3} \mathcal{P}\int_0^{+\infty} d\omega_k\, \omega_k^3 \left(\frac{1 + N(\omega_k)}{\omega - \omega_k} + \frac{N(\omega_k)}{\omega + \omega_k}\right)$$

$S(\omega)$ results from the density of bath modes. For a flat density one would have $S(\omega) = 0$

Examples: phonons bath
photon bath.

Exercise

Numerically solve

$$\frac{d\rho}{dt} = -i\,[H,\rho] + \kappa \sum_j \left(\hat{a}_j \rho a_j^\dagger - \frac{1}{2} a_j^\dagger a_j \rho - \frac{1}{2} \rho a_j^\dagger a_j\right)$$

$$H = \hbar\omega \sum_j a_j^\dagger a_j + J \sum_j \left(a_j a_{j+1}^\dagger + a_j^\dagger a_{j+1}\right)$$

$$+ U \sum_j a_j^{\dagger 2} a_j^2 + \sum_j \left(F e^{-i\omega_0 t} a_j^\dagger + F^* e^{i\omega_0 t} a_j\right)$$

Set $a_j^\dagger \leftarrow a_j^\dagger e^{-i\omega_0 t}$ $\quad a_j \leftarrow a_j e^{+i\omega_0 t}$

$$H = -\Delta \sum_j a_j^\dagger a_j + \; - - - \; + F \sum_j \left(a_j^\dagger + a_j\right)$$

$$\Delta, U, J, F \in \mathbb{R}$$

Define quantities wrt κ (i.e. set $\kappa = 1$)

Vectorization $\quad \rho \to |\rho\rangle$

$$|X\rho Y\rangle \to Y^T \otimes X\,|\rho\rangle$$

$$\mathcal{L} = -i\left(\mathbb{I} \otimes H - H^T \otimes \mathbb{I}\right) + \sum_j \left(a_j^* \otimes a_j - \frac{1}{2}\mathbb{I} \otimes a_j^\dagger a_j - a_j^T a_j^* \otimes \mathbb{I}\right)$$

For one boson,

$$a^{+} = \sum_{j=0}^{N_{max}-1} \sqrt{n+1}\, |n+1\rangle\langle n| = \begin{pmatrix} 0 & 1 & & & \\ & 0 & \sqrt{2} & & \\ & & 0 & \sqrt{3} & \\ & & & \ddots & \ddots \\ & & & & \sqrt{N_{max}} \end{pmatrix}$$

$\rho_s(t)$ is a statistical description of the state of the system.

Can we define a stochastic process for $|\psi(t)\rangle$ such that

$$\rho_s(t) = E\left(|\psi(t)\rangle\langle\psi(t)|\right)$$

"unravelling of the master equation"

Physical meaning: continuous measurement theory: stochastic dynamics produced by continuously monitoring a certain observable of the environment.

The stochastic process is then defined by a <u>piecewise deterministic process</u>

<u>Closed system</u>

$$U(t,t_0) = e^{-iH(t-t_0)}$$

$P[\psi, t] = P_0[U^{-1}(t,t_0)\psi]$

$P_0[x]$ initial PDF

If $P_0 = \delta(x) \Rightarrow |\psi(t)\rangle$ is fully deterministic.

A fully deterministic stoch process is per def Markov.

In terms of functional int.

$$P[\psi, t] = \int D\psi_0 D\psi_0^* \, P_0[\psi_0] \, \delta\left[\psi - U(t,t_0)\psi_0\right]$$

$$= P_0\left[U^{-1}(t,t_0)\psi_0\right]$$

Differential form

$$\frac{\delta}{\delta\psi(x)}\psi(y) = \frac{\delta}{\delta\psi^*(x)}\psi^*(y) = \delta(x-y)$$

$$\frac{\delta}{\delta\psi(x)}\psi^*(y) = \frac{\delta}{\delta\psi^*(x)}\psi(y) = 0$$

$$\frac{d}{dt}F(\psi(t)) = \int dx \left(\frac{\delta F}{\delta\psi(x)} \frac{d\psi(x,t)}{dt} + \frac{\delta F}{\delta\psi(x)^*} \frac{d\psi^*}{dt} \right)$$

$$\frac{\partial}{\partial t} P[\psi, t] = i \int dx \left\{ \frac{\delta}{\delta\psi(x)} (H\psi)(x) - \frac{\delta}{\delta\psi^*(x)} (H\psi)^*(x) \right\} \times P[\psi, t]$$

Liouville eq. corresp. to

$$\dot\psi(t) = -iH\psi(t)$$

Quantum master equation

$$\frac{d}{dt}\rho_s(t) = -i\left[H,\rho_s\right] + \sum_j \gamma_j\left(A_j\rho_s A_j^+ - \frac{1}{2}A_j^+A_j\rho_s - \frac{1}{2}\rho_s A_j^+A_j\right)$$

$$P[\Psi,t] = \int D\tilde{\Psi}D\tilde{\Psi}^* \, T[\Psi,t|\tilde{\Psi},t_0]\, P[\tilde{\Psi},t_0]$$

$$\rho_s(x,x',t) = E\left[\Psi(x,t)\Psi^*(x',t)\right] = \int D\Psi D\Psi^* \, P[\Psi,t]\,\Psi(x)\Psi^*(x')$$

We show that this Liouville eq. coincides with the QME

$$\frac{\partial}{\partial t}P[\Psi,t] = i\int dx\left(\delta_x G(\Psi)(x) - \delta_x^* G(\Psi)^*(x)\right)P[\Psi,t]$$

$$+\int D\tilde{\Psi}D\tilde{\Psi}^*\left(W[\Psi|\tilde{\Psi}]P[\tilde{\Psi},t] - W[\tilde{\Psi}|\Psi]P[\Psi,t]\right)$$

1st term:

$$\frac{d}{dt}\Psi(t) = -i\,G(\Psi(t))$$

$$= -i\tilde{H}\Psi(t) + \frac{1}{2}\sum_i \gamma_i \|A_i\Psi\|^2\Psi(t)$$

$$\tilde{H} = H - \frac{i}{2}\sum_j \gamma_j A_j^+A_j$$

$\tilde{H}$ is a non-hermitic Ham. implying a decay. ~~that~~

The nonlinear term in $G(\psi)$ is there to preserve the norm of ψ.

The eq. $\dot{\psi} = -i\,G(\psi)$ is then norm-preserving.

In the Liouville eq. there are gain and loss terms. The trans. rate is defined as

$$W(\psi|\tilde{\psi}) = \sum_j \gamma_j \|A_j\tilde{\psi}\|^2 \,\delta\!\left[\frac{A_j\tilde{\psi}}{\|A_j\tilde{\psi}\|} - \psi\right]$$

which defines jumps from ψ to $\dfrac{A_j\tilde{\psi}}{\|A_j\tilde{\psi}\|}$ with rates $\gamma_j\|A_j\tilde{\psi}\|^2$

Total trans rate from $\tilde{\psi}$: $\Gamma(\tilde{\psi})$

$$\Gamma(\tilde{\psi}) = \int D\psi D\psi^* \, W(\psi|\psi^*) = \sum_j \gamma_j \|A_j\tilde{\psi}\|^2$$

The formal solution between two jumps is $\psi(t) = \dfrac{e^{-i\tilde{H}t}\,\tilde{\psi}}{\| e^{-i\tilde{H}t}\,\tilde{\psi}\|}$

Deriving, one obtains $\dot{\psi} = -iG(\psi)$

So one can solve the linear Schr. eq. and take the norm at each time step.

To show that one obtains again the QME

$$\frac{\partial}{\partial t}\rho_s(x,x';t) = \int D\psi D\psi^* \frac{\partial}{\partial t} P(\psi,t)\,\psi(x)\psi^*(x') =$$

$$= \frac{\partial}{\partial t}\rho_s\Big|_L + \frac{\partial}{\partial t}\rho_s\Big|_J$$

$$\frac{\partial}{\partial t}\rho_s\Big|_L = i\int D\psi D\psi^* \int dy\, \psi(x)\psi^*(x') \times$$

$$\times \left\{ \frac{\delta}{\delta\psi(y)} G(\psi)(y) - \frac{\delta}{\delta\psi^*(y)} G(\psi)^*(y) \right\} P[\psi,t]$$

$$= -i\int D\psi D\psi^* \left\{ G(\psi)(x)\psi^*(x') - \psi(x) G^*(\psi)(x') \right\} P[\psi,t]$$

$$= -i\left[\tilde{H}, \rho_s\right] + \sum_j \gamma_j\, E\left[\|A_j\psi\|^2 \psi(x)\psi^*(x')\right]$$

$$\frac{\partial \rho_s}{\partial t}\Big|_J = \sum_j \gamma_j A_j \rho_s A_j^\dagger - \sum_j \gamma_j\, E\left[\qquad \right]$$

The sum

$$\frac{\partial}{\partial t}\rho_s = -i\left[\tilde{H}, \rho_s\right] + \sum_j \gamma_j A_j \rho_s A_j^+ \qquad \Box$$

Waiting time distr.

Total rate:

$$\Gamma(\tilde{\psi}) = \int D\psi D\psi^* \, W[\psi|\tilde{\psi}] =$$

$$= \sum_j \gamma_j \|A_j \tilde{\psi}\|^2$$

Suppose $\tilde{\psi}$ was reached with a jump at time t. At time $\tau \neq t$, rate of jumps

$$\Gamma[\psi(\tau)] = \sum_j \gamma_j \langle \psi(\tau)|A_j^+ A_j|\psi(\tau)\rangle$$

$$= -\frac{d}{d\tau} \ln \|e^{-i\tilde{H}\tau}\tilde{\psi}\|^2$$

In fact $\frac{d}{dt}\|e^{-i\tilde{H}t}\tilde{\psi}\|^2 = i\langle\tilde{\psi}|e^{i\tilde{H}^+t}(\tilde{H}^+ - \tilde{H})e^{-i\tilde{H}t}|\tilde{\psi}\rangle$

$$= -\sum_j \gamma_j \langle\tilde{\psi}|e^{i\tilde{H}^+t} A_j^+ A_j e^{-i\tilde{H}t}|\tilde{\psi}\rangle$$

but $\frac{e^{-i\tilde{H}t}|\tilde{\psi}\rangle}{\|e^{-i\tilde{H}t}\tilde{\psi}\|} = \psi(t)$. Then

$$\|e^{-i\tilde{H}t}\tilde{\psi}\|^{-2}\frac{d}{dt}\|e^{-i\tilde{H}t}\tilde{\psi}\|^2 = \sum_j \gamma_j \langle\psi(t)|A_j^+ A_j|\psi(t)\rangle$$

$W(\psi|\tilde{\psi})$ is the prob density per unit time of jumping from $\tilde{\psi}$ to ψ.
If before the jump the state is $\tilde{\psi}$, then there are a discrete set of possible trans.

$$\tilde{\psi} \to \psi = \frac{A_j \tilde{\psi}}{\|A_j \tilde{\psi}\|} \qquad p_j = \frac{\gamma_j \|A_j \tilde{\psi}\|^2}{\Gamma(\tilde{\psi})} \qquad \sum_j p_j = 1$$

These are the "quantum jumps".

We can translate the Liouville eq. into a stoch. diff. eq.

$$d\psi(t) = -i\, G(\psi(t)) + \sum_j \left(\frac{A_j \psi(t)}{\|A_j \psi(t)\|} - \psi(t) \right) dN_j(t)$$

$dN_j(t)$ stochastic Poisson increments

$$dN_j(t)\, dN_k(t) = \delta_{jk}\, dN_j(t)$$

$$E[dN_j(t)] = \gamma_j \|A_j \psi(t)\|^2 dt$$

the process $N_j(t)$ counts the number of jumps of type j. Its diff. $dN_j(t)$ defines the stoch process of the jumps of type j.

Stochastic dynamics in Hilbert space
Quantum Stochastic Differential Equation

$\rho(t)$ is a statistical description of the state of the system.

Can we define a stochastic process in Hilbert space $|\psi(t)\rangle$ such that

$$\rho(t) = \underline{E}\left(|\psi(t)\rangle\langle\psi(t)|\right)$$

This is possible in several different ways and it's called "unravelling of the master eq."

The physical meaning is that the stochastic dynamics is the result of continuous measurements of a certain observable of the environment. Each time the environment is measured, the full state of system + environment collapses into a tensor product state $|\psi(t)\rangle \otimes |\psi_E(t)\rangle$ which makes it possible to define $|\psi(t)\rangle$ at each t. The result is a (piecewise) deterministic process for $|\psi(t)\rangle$ called <u>quantum trajectory</u>

Several books an articles deal with this. See:

- Breuer - Petruccione "The theory of open quantum systems"
- Gardiner - Zoller "Quantum noise: ..."
- Wiseman - Milburn PRA 47, 1652 (1993)
- Plenio - Knight RMP 70, 101 (1998)
- Jacobs - Steck arXiv:quant-ph/0611067

⋮

Notice that the simplest QSDE is the Schrödinger equation:

$$d|\Psi(t)\rangle = -i H |\Psi(t)\rangle dt$$

this is non-stochastic. The corresponding master eq. is the von Neumann eq.

$$\frac{d\rho(t)}{dt} = -i[H, \rho(t)]$$

This, if interpreted as a stochastic process, is a Markovian process, because the evolution from time t is fully deterministic and thus only depends on the condition $\rho(t)$ and not on the past history.

Instead of deriving a general formal theory of QSDE, we will derive the ME from the QSDE in a very simple case, as an example. Then we will discuss all other cases briefly.

Consider a single bosonic mode subject to damping. The ME is

$$\frac{d\rho}{dt} = -i[H,\rho] - \frac{1}{2}\left(a^+a\rho + \rho a^+a - 2a\rho a^+\right)$$

We show that the stochastic diff. eq.

$$d|\Psi(t)\rangle = \left[dN(t)\left(\frac{a}{\sqrt{\langle n\rangle(t)}} - 1\right) + dt\left(\frac{\langle n\rangle(t)}{2} - \frac{a^+a}{2} - iH\right)\right]|\Psi(t)\rangle$$

is equivalent to the ME with $\rho(t) = E\left[|\Psi(t)\rangle\langle\Psi(t)|\right]$ provided $dN(t)$ is a random Poissonian number process, characterised by:

$$E\left[dN(t)\right] = \langle n\rangle(t)\,dt = \langle\Psi(t)|a^+a|\Psi(t)\rangle$$
$$= \mathrm{Tr}\left(a\,|\Psi(t)\rangle\langle\Psi(t)|\,a^+\right)$$

$(dN(t))^2 = dN(t)$ (random variable taking only values 0, 1)

Before we proceed, notice two things.

First, the QSDE is norm preserving, i.e. $\langle\Psi(t)|\Psi(t)\rangle = 1 \quad \forall t$

In general, if we have an unnormalized QSDE

$$d|\tilde{\Psi}\rangle = \left[A\,dt + (B-1)\,dN \right] |\tilde{\Psi}\rangle$$

The corresponding normalized QSDE is

$$d|\Psi\rangle = \left[\left(A - \frac{1}{2}\langle A + A^{+}\rangle\right) dt + \left(\frac{B}{\sqrt{\langle B^{+}B\rangle}} - 1\right) dN \right] |\Psi\rangle$$

We could use the unnormalized QSDE for our proof, but we would need to define

$$\rho(t) = E\left[\frac{|\tilde{\Psi}(t)\rangle\langle\tilde{\Psi}(t)|}{\langle\tilde{\Psi}(t)|\tilde{\Psi}(t)\rangle} \right]$$ instead.

The second remark is that the QSDE here is written in Itô form. We don't make here an intro to stochastic calculus. The main difference to ordinary calculus is the dependence of the increment on the integrand. In Itô:

$$\int_{t_0}^{t} g(t')\,dN(t') = \lim_{n \to \infty} \sum g(t_j)\left[N(t_{j+1}, 0) - N(t_j, 0) \right]$$

with $0 < t_1 < \dots < t_j$

First, for quantum variables, $[g(t'), dN(t')] = 0$ because the increment is at $t \geq t_j$ and is therefore uncorrelated to $dN(t_j)$ which only depends on $t < t_j$ (Markov)

However, for Itô, if a and b are stoch variables, then

$$d(ab) = a\,db + da\,b + da\,db$$

in fact, an SDE has the form

$$da = A\,dt + (B-1)\,dN$$

with $dN^2 \propto dt$ thus $dN \sim \sqrt{dt}$

If we want 1st order in dt of $d(ab)$ then we must include the dN^2 contrib from $da\,db$.

So rules for Itô calculus are different from ordinary calculus.

To avoid this there would be Stratonovich stochastic calculus, where the increment is defined as.

$$\int_{t_0}^{t} g(t')\,dN(t') = \lim_{n\to\infty}\left[\sum g(\bar{t}_j)\left[B(t_{j+1}) - B(\bar{t}_j)\right] + \right.$$
$$\left. + \sum g(\bar{t}_j)\left[B(\bar{t}_j) - B(t_j)\right]\right]$$

where $\bar{t}_j = \frac{1}{2}(t_j + t_{j+1})$

In this case the increment is $O(dt)$ and

$d(ab) = a\,db + da\,b$

but $[g(t'), dN(t')] \neq 0$. $\boxed{\text{We stick to Itô}}$

From the QSDE one has   let $\rho_c(t) = |\psi(t)\rangle\langle\psi(t)|$

$$d(|\psi\rangle\langle\psi|) = (d|\psi\rangle)\langle\psi| + |\psi\rangle d\langle\psi| + (d|\psi\rangle)(d\langle\psi|)$$

$$= \left[dN\left(\frac{a}{\sqrt{\langle n\rangle}} - 1\right) + dt\left(\frac{\langle n\rangle}{2} - \frac{n}{2} - iH\right)\right]\rho_c(t)$$

$$+ \rho_c(t)\left[dN\left(\frac{a^+}{\sqrt{\langle n\rangle}} - 1\right) + dt\left(\frac{\langle n\rangle}{2} - \frac{n}{2} + iH\right)\right]$$

$$+ dN(t)^2\left(\frac{a}{\sqrt{\langle n\rangle}} - 1\right)\rho_c(t)\left(\frac{a^+}{\sqrt{\langle n\rangle}} - 1\right)$$

Use $dN(t)^2 = dN(t)$ $n = a^+a$

$$d\rho_c(t) = dN(t)\left(\frac{a\rho_c a^+}{\langle n\rangle} - \rho_c\right) + dt\left(\langle n\rangle\rho_c - n\rho_c - \rho_c n - i[H,\rho_c]\right)$$

This is called stochastic master equation. and is still another stoch repr. of a Markovian OQS dynamics. Its property is to conserve purity, so if $\rho_c(0) = |\psi_0\rangle\langle\psi_0|$, then $\rho_c(t)$ is always a pure state

We now take the exp. value over the stat. ensemble.

Note that $E[dN(t)\rho_c(t)] = E[dN(t)]\,E(\rho_c(t))$ because of Markovianity $\rho_c(t)$ depends only on $dN(t')$ with $t' < t$.

Then

$$d\rho(t) = E\left[d\rho_c(t)\right]$$

$$= -i\left[H_{eff}, \rho\right]dt + a\rho a^{\dagger} dt$$

$$\Rightarrow \frac{d\rho}{dt} = -i\left[H_{eff}, \rho\right] + a\rho a^{\dagger}$$

$$H_{eff} = H - \frac{i}{2} a^{\dagger}a$$

which is the ME.

We can generalize to a stochastic rate γ by defining $E\left[dN(t)\right] = \gamma \langle n \rangle dt$

The process $dN(t)$ can be interpreted as a jump process, namely

$$dN(t) = \begin{cases} 1 & \text{if one boson is lost in } [t, t+dt] \\ 0 & \text{if not} \end{cases}$$

The generaliz. to several modes and decay channels is:

$$d|\psi(t)\rangle = \left(-i H_{eff} |\psi(t)\rangle + \frac{1}{2}\sum_j \gamma_j \langle\psi|A_j^{\dagger}A_j|\psi\rangle |\psi(t)\rangle\right)dt$$

$$+ \sum_j \left(\frac{A_j}{\langle\psi|A_j^{\dagger}A_j|\psi\rangle} - 1\right) dN_j(t)\, |\psi(t)\rangle$$

$$dN_j(t)\, dN_k(t) = \delta_{jk}\, dN_j(t)$$

$$E\left[dN_j(t)\right] = \gamma_j \langle\psi_j(t)| A_j^{\dagger}A_j |\psi_j(t)\rangle dt$$

and $\quad H_{eff} = H - \frac{i}{2} \sum_j \gamma_j A_j^\dagger A_j$

The interpretation in terms of quantum measurement here is that of "photodetection". We count quanta emitted into the environ. through the transition ("quantum jump") generated by a.

The total jump rate for the non-normalized $|\tilde{\Psi}(t)\rangle$ is

$$\Gamma(\tilde{\Psi}(t)) = \sum_j \gamma_j \langle \tilde{\Psi} | A_j^\dagger A_j | \tilde{\Psi} \rangle$$

From this one can show that, if a jump occurred at time t, the rate of the nex jump occurring at $t+\tau$ is

$$\Gamma[\Psi(t+\tau)] = -\frac{d}{d\tau} \ln \| e^{-iH_{eff}\tau} |\tilde{\Psi}(t)\rangle \|^2$$

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From $\Gamma(\psi(\tau))$ one can derive the distr function of the random waiting time τ as:

$$F[\tilde{\psi},\tau] = 1 - \exp\left(-\int_0^\tau ds\, \Gamma[\psi(\tau)]\right)$$

$$= 1 - \|\exp(-i\tilde{H}\tau)\tilde{\psi}\|^2$$

This is the prob that the next jump occurs between t and $t+\tau$

The stoch process $P[\psi,t]$ can therefore be simulated as follows:

1. Assume that the normalized state $\tilde{\psi}$ was reached at t.
2. Determine a random waiting time according to $F[\tilde{\psi},\tau]$. E.g. $\eta = \text{rand}(0,1)$ determine τ from

$$\eta = 1 - F(\tilde{\psi},\tau) = \|e^{-i\tilde{H}t}\tilde{\psi}\|^2$$

within $t, t+\tau$,

$$\psi(t+s) = \frac{e^{-i\tilde{H}s}\tilde{\psi}}{\|e^{-i\tilde{H}s}\tilde{\psi}\|} \qquad 0 \leq s \leq \tau$$

3. At time $t+\tau$ draw randomly one jump according to

$$p_j = \frac{\gamma_j \|A_j \psi(t+\tau)\|^2}{\sum_j \gamma_j \|A_j \psi(t+\tau)\|^2}$$

and replace

$$\psi(t+\tau) \to \frac{A_j \psi(t+\tau)}{\|A_j \psi(t+\tau)\|}$$

4 repeat 1 to 3

5 Average over several trajectories
$\psi^r(t) \quad r = 1, 2, \ldots, R$
obtained in this way.

Comments on Determining the waiting time

Diffusion limit of the Stoch Schr. eq.

$$A = \mathbb{I} + \varepsilon C \qquad \varepsilon \to 0$$

time density of trans arbitrarily large + $\varepsilon \to 0$

It can be shown that in this form one gets

$$d\psi(t) = -iK(\psi(t))dt + \sqrt{\bar{\gamma}_0}\, M(\psi(t))\, dW(t)$$

(in Ito form)

$dW(t)$ is the increment of a real Wiener process.

$$K(\psi) = H\psi + i\bar{\gamma}_0 \left\{ \langle C \rangle_\psi C - \frac{1}{2}\langle C \rangle_\psi^2 - \frac{1}{2} C^2 \right\} \psi$$

$$M(\psi) = \left(C - \langle C \rangle_\psi \right) \psi$$

$\bar{\gamma}_0 = \varepsilon^2 \gamma_0 \leftarrow$ rate.

$$dW_j(t)\, dW_{j'}(t') = \delta_{jj'}\, dt$$

Then $\langle (\Delta W)^2 \rangle = \Delta t$

and $\Delta W \propto \sqrt{\Delta t}$

Comments on efficiency of cont. meas.

The stoch. Dynamics that unravels the QME is not unique. E.g. $H, A_j, \gamma_j \to H', \gamma_j', A_j'$ will give a different stoch approach.

Interpretation as cont. measurement.

1 direct Photodetection → quantum jumps

2 Homodyne photodetection } stoch Schr. eq.
3 Heterodyne photodet. } with a Wiener Process.

Numerical methods for OQS: overview

We may need to solve one of two problems:

1. Dynamics: $\dot{\rho} = \mathcal{L}\rho$
2. NESS: $\mathcal{L}\rho = 0$ with $\mathrm{Tr}(\rho) = 1$

Remarks:

- Liouvillian super-operator $\mathcal{L}$ is non-hermitian
  has complex eigenvalues. If λ is ev. λ^* is.
  Some ev are real only

  $Re(\lambda) \leq 0$ dissipative dynamics

  $Re(\lambda) = 0$ NESS.

  Existence and/or unicity of NESS
  is not obvious or granted!

  D. Nigro, arXiv: 1803.06279

  F. Minganti et al. arXiv: 1804.11293

- To numerically solve, it is almost always
  useful to adopt Choi isomorphism, aka
  vectorization. Map operators on $\mathcal{H}$ to
  vectors on $\mathcal{H} \otimes \mathcal{H}$

$$\rho = \sum_{jk} \rho_{jk} |j\rangle\langle k| \longrightarrow |\rho\rangle = \sum_{jk} \rho_{jk} |j\rangle \otimes |k\rangle$$

i.e. concatenate the columns of ρ.

For vectorization, given operators X, Y;

$$|X\rho Y\rangle \to (Y^T \otimes X)|\rho\rangle$$

Then the Liouvillian is mapped onto the op.

$$\mathcal{L} = -i\left(\mathbb{I} \otimes H - H^T \otimes \mathbb{I}\right) + \sum_j \left[A_j^* \otimes A_j - \frac{1}{2}\mathbb{I} \otimes A_j^\dagger A_j - A_j^T A_j^* \otimes \mathbb{I}\right]$$

which can be built directly into computer code.

Review: Weimer et al. arXiv:1907.07079

1) - We have already seen QSDE

Pro: $O(N)$ instead of $O(N^2)$

Con: May not sample efficiently

Difficulty in solving SDE

- Exact method.

Choose a finite-dim Hilbert space (for Bosons, truncate to N_{max}/site)

Solve $\dot{\rho} = \mathcal{L}\rho$ as a (nonlinear) ODE.

Pro: Direct solution, exact up to truncation

Con: $O(N^2)$ mostly memory limitations.

- MPO / TEBD

Based on the idea of decomposing $|\rho\rangle$ as an MPS or ρ as an MPO an applying Trotter decomposition to $\mathcal{L}$.

<u>Pro</u>: Very efficient for small bond dimension (which is often the case in dissipative systems)
$\mathcal{O}(N) \rightarrow \mathcal{O}(D^4 \times d^2 \times N_{sites})$

<u>Con</u>: • Inefficient if transient is highly quantum correlated
• You must be well motivated as it is hard to code
https://www.tensors.net
• Only 1D. 2D is a mess

- Approximate methods
Cluster mean-field
Stochastic Gutzwiller
Phase-space Methods (TWA)

<u>Pro</u>: Fast. not memory demanding
<u>Con</u>: Approx is always uncontrolled

(2) $\mathcal{L}\rho = 0 \quad Tr(\rho) = 1$

For finite-dim Hilbert space usually 1 only $\lambda = 0$ NESS.

- Exact:
  Solve $\mathcal{L}\rho = 0$ with cond $Tr(\rho) = 1$
  Lagrange multipliers
  More easily, replace 1^{st} line of $\mathcal{L}$ with condition $Tr(\rho) = 1$ (inh system)
  <u>Pro</u>: Exact accurate
  <u>Con</u>: $O(N^2)$
  Sometimes the system is difficult as $\mathcal{L}$ is bad conditioned.
  Use convergence methods lsqr bicg etc. Never good to use eigs.

- Corner space renormalization
  Finazzi et al. arXiv: 1502.05651
  <u>Idea</u>:

$$\rho_1 \xleftrightarrow{J} \rho_2$$

$$\rho_1 = \sum_j p_{1,j} |\varphi_{1,j}\rangle\langle\varphi_{1,j}| \qquad \rho_2 = \sum_j p_{2,j} |\varphi_{2,j}\rangle\langle\varphi_{2,j}|$$

Take M highest values among $\{ p_{1,j} \times p_{2,k} \}$

Write all operators on the "basis"

$\{ |\varphi_{1,j}\rangle \otimes |\varphi_{2,k}\rangle$, k,j in the corner space $\}$

Solve $\mathcal{L}\rho = 0$ for system $1+2$
on the corner space

Iterate.

Pro: Can be super efficient with very small M.

Con: Careful coding.
Works only for weakly entropic systems, as M grows with
$S = \mathrm{Tr}(\rho \ln \rho)$

- Variational QMC with neural network

Nagy, VS, arXiv:1902.09483

Hartmann, Carleo arXiv:1902.05131

Vicentini et al. arXiv:1902.10104

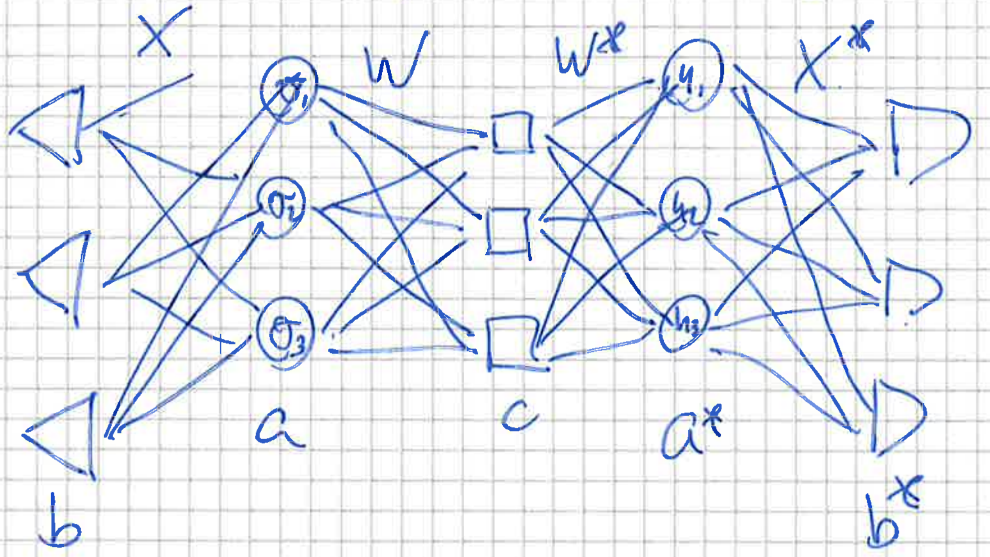
Yoshioka et al. arXiv:1902.07006

variational principle $\dfrac{\| \mathcal{L}|\rho\rangle \|^2}{\| |\rho\rangle \|^2}$ or

Real time QMC evolution with SR

TN ansatz RBM (pos. defined)

$$\rho_X(\sigma,\eta) = \exp\left(\sum a_i \sigma_i\right) \exp\left(\sum a_i^* \eta_i\right)$$
$$\times \prod_{\ell=1}^{L} \cosh\left(c_\ell + \sum_i W_{\ell i}\sigma_i + \sum_i W_{\ell i}^* \eta_i\right)$$
$$\times \prod_{m=1}^{M} \cosh\left(b_m + \sum_i X_{mi}\sigma_i\right)$$
$$\times \prod_{u=1}^{M} \cosh\left(b_u^* + \sum_i X_{ui}^* \eta_i\right)$$



Solve using SR (real time dynamics)
or minimize L^+L with conj gr.
Sample values using Metropolis-Hastings
QMC.

<u>Pro</u>: $O(\text{poly}(N_{\text{sites}}))$ and indep. of dimension.

<u>Con</u>: MC, control param non physic. mean.

- Variational MPO

Mascarenhas Savona, arXiv: 1504.06127

Cui et al. arXiv: 1501.06786

again repres. ρ as MPO

variational sol with DMRG

Pro: $O(\text{poly}(N_{\text{sites}}))$ very efficient if poor entanglement

Con: 1D, non-positive.