A hopefully gentle (but not rigorous) derivation of Lindblad equation

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Math preparations

An important identity:

$$(A \otimes B)(C \otimes D) = AC \otimes BD \tag{1}$$

this will be used multiple times in derivation.

eom of density matrix reads

$$\begin{aligned} &\dot{\rho(t)} = -\frac{i}{\hbar}[H, \rho] \\ &\Leftrightarrow \dot{\rho(t)} = \mathcal{L}\rho, \end{aligned} \tag{2}$$

where $\mathcal{L} = -\frac{i}{\hbar}[H, (\cdot)]$.

In the so-called Liouville space, density matrix ρ is vectorized: $\rho \to |\rho\rangle\rangle$, and $\mathcal{L}$ is a matrix that acts on a matrix $\mathcal{L} \to \hat{\hat{\mathcal{L}}}$, which is called superoperator.

Liouville space and all related algebra do not introduce new physics, it's merely a mathematical trick, to make use of linear algebra techniques.

Let $\{|i\rangle|\ i = 1.2.\cdots\}$ be orthonormal basis, then operator $\hat{\rho}$ can be decomposed as

$$\hat{\rho} = \sum_{i,j} |i\rangle\langle i|\hat{\rho}|j\rangle\langle j| = \sum_{i,j} \rho_{ij} |i\rangle\langle j|, \tag{3}$$

which is equivalent to a vectorized form

$$\sum_{ij} \rho_{ij} |i\rangle\langle j| \Leftrightarrow \sum_{ij} \rho_{ij}\ |i\rangle \otimes |j\rangle \tag{4}$$

and matrix acting on it can be rewritten as

$$
\begin{aligned}
&H\ |\rho\rangle\rangle = \sum \rho_{ij} H|i\rangle \otimes |j\rangle \equiv \sum \rho_{ij} H \otimes I\ |i\rangle \otimes |j\rangle \\
&\Rightarrow H\ |\rho\rangle\rangle = H \otimes I\ |\rho\rangle\rangle
\end{aligned}
$$

$$
\begin{aligned}
&\rho H = \sum \rho_{ij}|i\rangle\langle j|H = \sum_{ij} \rho_{ij}|i\rangle\big(H^\dagger\ |j\rangle\big)^\dagger \equiv \sum \rho_{ij}|i\rangle \otimes H^\dagger|j\rangle \equiv \sum \rho_{ij} I \otimes H^\dagger|i\rangle \otimes |j\rangle \\
&\Rightarrow I \otimes H^\dagger\ |\rho\rangle\rangle
\end{aligned}
\tag{5}
$$

$$
H\rho - \rho H = [H,\rho]_- \equiv \big(H \otimes I - I \otimes H^\dagger\big)|\rho\rangle\rangle
$$

Therefore the Liouville superoperator is

$$
\mathcal{L} = -\frac{i}{\hbar}[H,(\cdot)] = -\frac{i}{\hbar}(H \otimes I - I \otimes H) \tag{6}
$$

and $\mathcal{L}|\rho\rangle\rangle = -\frac{i}{\hbar}(H \otimes I - I \otimes H)\ |\rho\rangle\rangle$.

This is how Liouville superoperator is constructed in practice.

The construction of anti-commutator superoperator is similar: $\{s^\dagger s,(\cdot)\}_+ = s^\dagger s \otimes I + I \otimes s^\dagger s$. Another type is $s\rho s^\dagger$, which can be constructed by

$$
\begin{aligned}
s\rho s^\dagger &= \sum \rho_{ij} s|i\rangle\langle j|s^\dagger \\
&= \sum \rho_{ij} s|i\rangle(s|j\rangle)^\dagger \\
&\equiv \sum \rho_{ij} s|i\rangle \otimes s|j\rangle \\
&= s \otimes s\ |\rho\rangle\rangle
\end{aligned}
\tag{7}
$$

In summary

$[H,(\cdot)]_-$	$\{s^\dagger s,(\cdot)\}_+$	$s(\cdot)s^\dagger$
$H \otimes I - I \otimes H$	$s^\dagger s \otimes I + I \otimes s^\dagger s$	$s \otimes s$

Lindbladian

Hamiltonian is factored into two parts $H = H^0 + H'(t)$, where H^0 is easily solvable and all difficult parts are absorbed into $H'(t)$. The eom of density matrix under interaction picture is given by

$$
\begin{aligned}
\dot{\rho_I^{tot}} &= \frac{\partial}{\partial t}\Big(e^{i\frac{H^0 t}{\hbar}}\rho_S^{tot}e^{-i\frac{H^0 t}{\hbar}}\Big) \\
&= \frac{iH^0}{\hbar}e^{\frac{iH^0 t}{\hbar}}\rho e^{-i\frac{H^0 t}{\hbar}} + e^{\frac{iH^0 t}{\hbar}}\dot{\rho}e^{-i\frac{H^0 t}{\hbar}} - e^{\frac{iH^0 t}{\hbar}}\rho\frac{iH^0}{\hbar}e^{-i\frac{H^0 t}{\hbar}} \\
\dot{\rho_I^{tot}}(t) &= \frac{i}{\hbar}e^{\frac{iH^0 t}{\hbar}}H^0\rho e^{-i\frac{H^0 t}{\hbar}} - \frac{i}{\hbar}e^{\frac{iH^0 t}{\hbar}}[H^0+H',\rho]e^{-i\frac{H^0 t}{\hbar}} - e^{\frac{iH^0 t}{\hbar}}\rho e^{-i\frac{H^0 t}{\hbar}}\frac{iH^0}{\hbar} \\
&= \frac{i}{\hbar}H_I^0\rho_I^{tot} - \frac{i}{\hbar}e^{\frac{iH^0 t}{\hbar}}H^0\rho e^{-i\frac{H^0 t}{\hbar}} - \frac{i}{\hbar}e^{\frac{iH^0 t}{\hbar}}H'\rho e^{-i\frac{H^0 t}{\hbar}} + \frac{i}{\hbar}e^{\frac{iH^0 t}{\hbar}}\rho H^0 e^{-i\frac{H^0 t}{\hbar}} + e^{\frac{iH^0 t}{\hbar}}\rho H' e^{-i\frac{H^0 t}{\hbar}} - \rho_I^{tot}H_I^0\frac{i}{\hbar} \\
&= \frac{i}{\hbar}\big(H_I^0\rho_I^{tot} - H_I^0\rho_I^{tot} - H_I'\rho_I^{tot} + \rho_I^{tot}H_I^0 + \rho_I^{tot}H_I' - \rho_I^{tot}H_I^0\big) \\
&= -\frac{i}{\hbar}[H_I'(t), \rho_I^{tot}(t)]
\end{aligned} \tag{8}
$$

Under interation picture, the eom of density matrix has the same form as that under Schrodinger picture.

Since density matrix is time-dependent, the formal solution to its eom involves time-ordering

$$
\begin{aligned}
&\rho_I^{tot}(t) - \rho_I^{tot}(0) = -\frac{i}{\hbar}\int_0^t [H_I'(t'), \rho_I^{tot}(t')]dt' \\
&\rho_I^{tot}(t) = \rho_I^{tot}(0) - \frac{i}{\hbar}\int_0^t\left[H_I'(t'), \rho_I^{tot}(0) - \frac{i}{\hbar}\int_0^{t'}[H_I'(t''), \rho_I^{tot}(t'')]dt''\right]dt' \\
&\vdots
\end{aligned} \tag{9}
$$

The expansion stops at the second order:

$$
\rho_I^{tot}(t) = \rho_I^{tot}(0) - \frac{i}{\hbar}\int_0^t [H_i'(t'), \rho_I^{tot}(0)]dt' - \frac{1}{\hbar^2}\int_0^t dt'\left[H_I'(t'), \int_0^{t'}[H_I'(t''), \rho_I^{tot}(t'')]dt''\right] \tag{10}
$$

Taking time derivative to get rid of one integral

$$
\dot{\rho_I^{tot}}(t) = -\frac{i}{\hbar}[H_I'(t), \rho_I^{tot}(0)] - \frac{1}{\hbar^2}\int_0^t [H_I'(t), [H_I'(t'), \rho_I^{tot}(t')]]dt' \tag{11}
$$

So far, no approximations are made. We assume the system and bath are weakly coupled, thus the total density matrix is approximately a direct product of system density matrix and bath density matrix: $\rho_I^{\text{tot}}(t) \approx \rho_I^S(t) \otimes \rho_I^B(t)$; and we assume the bath is too large to be affected: $\rho_I^B(t) = \rho_I^B(0) = R_0$, therefore $\rho_I^{\text{tot}}(t) = \rho_I^S(t) \otimes R_0$.

The total Hamiltonian reads $H = H_S + H_B + H'$, where H_S and H_B act solely on system and bath, while the coupling part H' acts on both. This writing is misleading as the Hamiltonian is actually direct product:

$$
\begin{aligned}
&H_S = H_S \otimes I \\
&H_S\rho^{\text{tot}} = H_S \otimes I\rho_S \otimes \rho_B = H_S\rho_S \otimes \rho_B \\
\\
&H_B = I \otimes H_B \\
&H_B\rho^{\text{tot}} = I \otimes H_B\rho_S \otimes \rho_B = \rho_S \otimes H_B\rho_B \\
\\
&H' = s \otimes \Gamma \\
&H'\rho^{\text{tot}} = s\rho_S \otimes \Gamma\rho_B,
\end{aligned}
\tag{12}
$$

where s and Γ are system and bath operator, respectively. Under interaction picture, s and Γ are transformed accordingly

$$
\begin{aligned}
&s \rightarrow \tilde{s} \\
&\Gamma \longrightarrow \tilde{\Gamma} \\
&H_I' = \tilde{s} \otimes \tilde{\Gamma}
\end{aligned}
\tag{13}
$$

To get the information of system, we trace out the bath part:

$$
\begin{aligned}
&\dot{\rho_{S,I}}(t) = \mathrm{Tr}_B\dot{\rho_I^{\text{tot}}}(t) \\
&= -\frac{i}{\hbar}\mathrm{Tr}_B\big\{H_I'(t)\rho_I^S(0) \otimes R_0 - \rho_I^S(0) \otimes R_0H_I'(t)\big\} - \frac{1}{\hbar^2}\mathrm{Tr}_B\int_0^t [H_I'(t), [H_I'(t'), \rho_I^{tot}(t')]]dt' \\
&= -\frac{i}{\hbar}\big(\tilde{s}(t)\rho_I^S(0)\mathrm{Tr}_B\big\{\tilde{\Gamma}(t)R_0\big\} - \rho_I^S(0)\tilde{s}(t)\mathrm{Tr}_B\big\{R_0\tilde{\Gamma}(t)\big\}\big) - \cdots
\end{aligned}
\tag{14}
$$

Here $\mathrm{Tr}_B\big\{R_0\tilde{\Gamma}(t)\big\}$ is the expectation value of bath, we assume it to be zero. Then

$$
\dot{\rho_{S,I}}(t) = \mathrm{Tr}_B\dot{\rho_I^{\text{tot}}}(t) = -\frac{1}{\hbar^2}\mathrm{Tr}_B\int_0^t [H_I'(t), [H_I'(t'), \rho_I^{tot}(t')]]dt', \tag{15}
$$

which states the state of system at time t is related to the state of system at time t' that is prior to t. If the thermal-equilibrium of bath is much faster than the evolution of system, the state of system is not determined by its history, so we get

$$
\dot{\rho_{S,I}}(t) = -\frac{1}{\hbar^2}\mathrm{Tr}_B\int_0^t [H_I'(t), [H_I'(t'), \rho_I^{tot}(t)]]dt' \tag{16}
$$

Interaction Haimltonian is direct product of system operator and bath operator $H' = \hbar\sum_i s_i \otimes \Gamma_i$, and under interation picture it has the same form $H_I' = \hbar\sum_i \tilde{s}_i \otimes \tilde{\Gamma}_i$. So Equation 16 can be further simplified:

$$
\begin{aligned}
\dot{\rho_{S,I}}(t) &= -\frac{1}{\hbar^2}\int_0^t \mathrm{Tr}_B\left[\hbar\sum_i \tilde{s}_i(t) \otimes \tilde{\Gamma}_i(t), \left[\hbar\sum_j \tilde{s}_j(t') \otimes \widetilde{\Gamma_j}(t'), \rho_i^{\text{tot}}(t)\right]\right]dt' \\
&= -\sum_{ij}\int_0^t \mathrm{Tr}_B\left[\tilde{s}_i(t) \otimes \tilde{\Gamma}_i(t), \tilde{s}_j(t') \otimes \widetilde{\Gamma_j}(t')\rho_I^{\text{tot}}(t) - \rho_I^{\text{tot}}(t)\tilde{s}_j(t') \otimes \widetilde{\Gamma_j}(t')\right]dt'
\end{aligned}
\tag{17}
$$

Toal density matrix is approximately direct product of system density matrix and bath density matrix: $\rho_I^{\text{tot}}(t) \approx \rho_{S,I}(t) \otimes \rho_{B,I}(t) = \rho_{S,I}(t) \otimes R_0$. So

$$
\begin{aligned}
\dot{\rho_{S,I}}(t) = -\sum_{ij}\int_0^t \mathrm{Tr}_B\Big\{ & \tilde{s}_i(t)\otimes\tilde{\Gamma}_i(t)\tilde{s}_j(t')\otimes\widetilde{\Gamma}_j(t')\rho_{S,I}(t)\otimes R_0 \\
& -\tilde{s}_i(t)\otimes\tilde{\Gamma}_i(t)\rho_{S,I}(t)\otimes R_0\tilde{s}_j(t')\otimes\widetilde{\Gamma}_j(t') \\
& -\tilde{s}_j(t')\otimes\widetilde{\Gamma}_j(t')\rho_{S,I}(t)\otimes R_0\tilde{s}_i(t)\otimes\tilde{\Gamma}_i(t) \\
& +\rho_{S,I}(t)\otimes R_0\tilde{s}_j(t')\otimes\widetilde{\Gamma}_j(t')\tilde{s}_i(t)\otimes\tilde{\Gamma}_i(t)\Big\}dt'
\end{aligned}
\tag{18}
$$

$$
\begin{aligned}
\dot{\rho_{S,I}}(t) = & -\sum_{ij}\int_0^t \mathrm{Tr}_B\Big\{ \\
& \Big(\tilde{s}_i(t)\tilde{s}_j(t')\otimes\tilde{\Gamma}_i(t)\widetilde{\Gamma}_j(t')\Big)\rho_{S,I}(t)\otimes R_0 \\
& -\big(\tilde{s}_i(t)\rho_{S,I}(t)\otimes\tilde{\Gamma}_i(t)R_0\big)\tilde{s}_j(t')\otimes\widetilde{\Gamma}_j(t') \\
& -\Big(\tilde{s}_j(t')\rho_{S,I}(t)\otimes\widetilde{\Gamma}_j(t')R_0\Big)\tilde{s}_i(t)\otimes\tilde{\Gamma}_i(t) \\
& +\Big(\rho_{S,I}(t)\tilde{s}_j(t')\otimes R_0\widetilde{\Gamma}_j(t')\Big)\tilde{s}_i(t)\otimes\tilde{\Gamma}_i(t)\Big\}dt' \\
& = -\sum_{ij}\int_0^t \mathrm{Tr}_B\Big\{ \\
& \tilde{s}_i(t)\tilde{s}_j(t')\rho_{S,I}(t)\otimes\tilde{\Gamma}_i(t)\widetilde{\Gamma}_j(t')R_0 \\
& -\tilde{s}_i(t)\rho_{S,I}(t)\tilde{s}_j(t')\otimes\tilde{\Gamma}_i(t)R_0\widetilde{\Gamma}_j(t') \\
& -\tilde{s}_j(t')\rho_{S,I}(t)\tilde{s}_i(t)\otimes\widetilde{\Gamma}_j(t')R_0\tilde{\Gamma}_i(t) \\
& +\rho_{S,I}(t)\tilde{s}_j(t')\tilde{s}_i(t)\otimes R_0\widetilde{\Gamma}_j(t')\tilde{\Gamma}_i(t)\Big\}dt' \\
& = -\sum_{ij}\int_0^t \langle\tilde{\Gamma}_i(t)\widetilde{\Gamma}_j(t')\rangle\big(\tilde{s}_i(t)\tilde{s}_j(t')\rho_{S,I}(t)-\tilde{s}_j(t')\rho_{S,I}(t)\tilde{s}_i(t)\big) \\
& -\langle\widetilde{\Gamma}_j(t')\tilde{\Gamma}_i(t)\rangle\big(\tilde{s}_i(t)\rho_{S,I}(t)\tilde{s}_j(t')-\rho_{S,I}(t)\tilde{s}_j(t')\tilde{s}_i(t)\big)dt',
\end{aligned}
\tag{19}
$$

where $\langle\tilde{\Gamma}_i(t)\widetilde{\Gamma}_j(t')\rangle$ is the correlation function of bath operator. Correlation between different bath operators is zero; correlation within the same bath operator behaves like delta function:

$$
\langle\tilde{\Gamma}_i(t)\widetilde{\Gamma}_j(t')\rangle \propto \delta_{ij}\delta(t-t')
\tag{20}
$$

System operators are hermitian. Replacing s_i in the first term with $s_i^\dagger$, and s_j with $s_j^\dagger$ in the second term renders

$$
\begin{aligned}
\dot{\rho_{S,I}}(t) = -\sum_{ij}\int_0^t & \langle\tilde{\Gamma}_i(t)\widetilde{\Gamma}_j(t')\rangle\left(\tilde{s_i^\dagger}(t)\tilde{s}_j(t')\rho_{S,I}(t)-\tilde{s}_j(t')\rho_{S,I}(t)\tilde{s_i^\dagger}(t)\right) \\
& -\langle\widetilde{\Gamma}_j(t')\tilde{\Gamma}_i(t)\rangle\left(\tilde{s}_i(t)\rho_{S,I}(t)\tilde{s_j^\dagger}(t')-\rho_{S,I}(t)\tilde{s_j^\dagger}(t')\tilde{s}_i(t)\right)
\end{aligned}
\tag{21}
$$

If the system operator satisfies

$$
\begin{aligned}
\left[H_{\text{sys}}, s_i\right] &= -\hbar\omega_i s_i \\
\left[H_{\text{sys}}, s_i^\dagger\right] &= \hbar\omega_i s_i^\dagger,
\end{aligned}
\tag{22}
$$

for example the system Hamiltonian is qho without zpe and system operator is creation/annihilation operator, then under interaction picture system operator reads

$$
\begin{aligned}
\tilde{s_i} &= e^{i\frac{H_{\text{sys}}}{\hbar}t} s_i e^{-i\frac{H_{\text{sys}}}{\hbar}t} \\
\tilde{s_i^\dagger} &= e^{i\frac{H_{\text{sys}}}{\hbar}t} s_i^\dagger e^{-i\frac{H_{\text{sys}}}{\hbar}t}
\end{aligned}
\tag{23}
$$

Here comes operator exponential $e^A B e^{-A}$, and Baker-Hausdorff formula states

$$
e^A B e^{-A} = B + [A, B] + \frac{1}{2!}[A, [A, B]] + \frac{1}{3!}[A, [A, [A, B]]] + \cdots \tag{24}
$$

Proof. Let $F(\lambda) = e^{\lambda A} B e^{-\lambda A}$, its Taylor expansion at $\lambda = 0$ is:

$$
\begin{aligned}
&F'(\lambda)|_{\lambda=0} = \left(Ae^{\lambda A}Be^{-\lambda A} - e^{\lambda A}Be^{-\lambda A}A\right)|_{\lambda=0} = (AF - FA)|_{\lambda=0} = [A, B] \\
&F''(\lambda)|_{\lambda=0} = (AF' - F'A)|_{\lambda=0} = [A, [A, F]]|_{\lambda=0} = [A, [A, B]] \\
&F'''(\lambda)|_{\lambda=0} = (AF'' - F''A)|_{\lambda=0} = (A[A, [A, F]] - [A, [A, F]]A)|_{\lambda=0} = [A, [A, [A, F]]] = [A, [A, [A, B]]] \\
&\vdots
\end{aligned}
$$

Finally let $\lambda = 1$. $\square$

Then the system operators s_i and $s_i^\dagger$ under interaction picture look like

$$
\begin{aligned}
\tilde{s_i} &= s_i + \left(-\hbar\omega_i \frac{it}{\hbar}\right) s_i + \frac{\left(\left(-\hbar\omega_i \frac{it}{\hbar}\right)\right)^2}{2!} s_i + \frac{\left(\left(-\hbar\omega_i \frac{it}{\hbar}\right)\right)^3}{3!} s_i + \cdots = e^{-i\omega_i t} s_i \\
\tilde{s_i^\dagger} &= e^{i\omega_i t} s_i^\dagger
\end{aligned}
\tag{25}
$$

Combine Equation 21, Equation 20, and Equation 25 together, and let γ_i depict the coupling strength, we get

$$
\begin{aligned}
&\dot{\rho_{S,I}}(t) = -\sum_i \int_0^t \gamma_i \delta(t - t') \Big(\tilde{s_i^\dagger}(t)\tilde{s_i}(t')\rho_{S,I}(t) - \tilde{s_i}(t')\rho_{S,I}(t)\tilde{s_i^\dagger}(t) \\
&-\tilde{s_i}(t)\rho_{S,I}(t)\tilde{s_i^\dagger}(t') + \rho_{S,I}(t)\tilde{s_i^\dagger}(t')\tilde{s_i}(t)\Big) dt' \\
&= -\sum_i \int_0^t \gamma_i \delta(t - t') \big(s_i^\dagger(t)s_i(t')\rho_{S,I}(t)e^{i\omega_i(t-t')} - s_i(t')\rho_{S,I}(t)s_i^\dagger(t)e^{i\omega_i(t-t')} \\
&-s_i(t)\rho_{S,I}(t)s_i^\dagger(t')e^{i\omega_i(t'-t)} + \rho_{S,I}(t)s_i^\dagger(t')s_i(t)\big)e^{i\omega_i(t'-t)} dt'
\end{aligned}
\tag{26}
$$

Note that $\int_0^t e^{i\omega(t-\tau)}\delta(t-\tau)d\tau = \frac{1}{2}$, then

$$
\begin{aligned}
&\dot{\rho_{S,I}}(t) = -\sum_i \frac{\gamma_i}{2}\left(s_i^\dagger(t)s_i(t)\rho_{S,I}(t) - s_i(t)\rho_{S,I}(t)s_i^\dagger(t) - s_i(t)\rho_{S,I}(t)s_i^\dagger(t) + \rho_{S,I}(t)s_i^\dagger(t)s_i(t)\right) \\
&= -\sum_i \frac{\gamma_i}{2}\left(\left\{s_i^\dagger(t)s_i(t), \rho_{S,I}(t)\right\} - 2s_i(t)\rho_{S,I}(t)s_i^\dagger(t)\right)
\end{aligned}
\tag{27}
$$

This is how bath affects the dynamics of system density matrix. Going back to Schrodinger picture, and adding on unitary part finally gives

$$\dot{\rho_{S,S}}(t) = -\frac{i}{\hbar}\left[H_{\text{sys}}, \rho_{S,S}\right]_{-} - \sum_i \frac{\gamma_i}{2}\left(\left\{s_i^\dagger s_i, \rho_{S,S}\right\}_{+} - 2s_i\rho_{S,S}s_i^\dagger\right) \tag{28}$$