Open quantum systems – lecture 12

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4.2 Pure-dephasing spin-boson model

We consider the total Hamiltonian

$$H = \Omega\sigma^z + \sigma^z \otimes \sum_k (h_k b_k + h_k^* b_k^\dagger) + \sum_k \omega_k b_k^\dagger b_k \,. \tag{4.1}$$

Since the interaction commutes with the system Hamiltonian, the energy of the system will remain constant. We can apply the so-called **polaron transformation** (also: Lang-Firsov transform [1]) to the whole Hamiltonian

$$U = \exp\left\{-\sigma^z \sum_k \left(\frac{h_k}{\omega_k} b_k - \frac{h_k^*}{\omega_k} b_k^\dagger\right)\right\} . \tag{4.2}$$

We note the following relations

$$\begin{aligned} U\sigma^z U^\dagger &= \sigma^z \,, \\ U\sigma^\pm U^\dagger &= e^{\pm 2\sum_k \left(\frac{h_k^*}{\omega_k} b_k^\dagger - \frac{h_k}{\omega_k} b_k\right)} \sigma^\pm \,, \\ U b_k U^\dagger &= b_k - \frac{h_k^*}{\omega_k}\sigma^z \,, \end{aligned} \tag{4.3}$$

which can e.g. be shown using the Lee expansion formula. From this we conclude that in the Schrödinger picture

$$\begin{aligned} UHU^\dagger &= \Omega\sigma^z + \sigma^z \sum_k \left(h_k b_k + h_k^* b_k^\dagger - 2\frac{|h_k|^2}{\omega_k}\sigma^z\right) + \sum_k \omega_k \left(b_k^\dagger - \frac{h_k}{\omega_k}\sigma^z\right)\left(b_k - \frac{h_k^*}{\omega_k}\sigma^z\right) \\ &= \Omega\sigma^z - \sum_k \frac{|h_k|^2}{\omega_k} + \sum_k \omega_k b_k^\dagger b_k \,. \end{aligned} \tag{4.4}$$

This means that in this frame, the evolution of spin and boson are completely decoupled. Consequently, we can e.g. compute the expectation value of σ^α via

$$\begin{aligned} \langle\sigma^\alpha\rangle &= \mathrm{Tr}\left\{e^{+\mathrm{i}Ht}\sigma^\alpha e^{-\mathrm{i}Ht}\rho_0\right\} = \mathrm{Tr}\left\{U^\dagger U e^{+\mathrm{i}Ht} U^\dagger U \sigma^\alpha U^\dagger U e^{-\mathrm{i}Ht} U^\dagger U \rho_0\right\} \\ &= \mathrm{Tr}\left\{U^\dagger e^{+\mathrm{i}UHU^\dagger t} U\sigma^\alpha U^\dagger e^{-\mathrm{i}UHU^\dagger t} U\rho_0\right\} \\ &= \mathrm{Tr}\left\{U^\dagger e^{+\mathrm{i}\Omega t\sigma^z} e^{+\mathrm{i}\sum_k \omega_k t b_k^\dagger b_k} U\sigma^\alpha U^\dagger e^{-\mathrm{i}\sum_k \omega_k t b_k^\dagger b_k} e^{-\mathrm{i}\Omega t\sigma^z} U\rho_0\right\} . \end{aligned} \tag{4.5}$$

For $\alpha = +$ we further calculate

$$
\begin{aligned}
\left\langle\sigma^+\right\rangle &= \mathrm{Tr}\left\{U^\dagger e^{+\mathrm{i}\sum_k \omega_k t b_k^\dagger b_k} e^{2\sum_k\left(\frac{h_k^*}{\omega_k}b_k^\dagger - \frac{h_k}{\omega_k}b_k\right)} e^{-\mathrm{i}\sum_k \omega_k t b_k^\dagger b_k} e^{+\mathrm{i}\Omega t\sigma^z}\sigma^+ e^{-\mathrm{i}\Omega t\sigma^z} U\rho_0\right\}\\
&= e^{+2\mathrm{i}\Omega t}\mathrm{Tr}\left\{U^\dagger e^{2\sum_k\left(\frac{h_k^*}{\omega_k}b_k^\dagger e^{+\mathrm{i}\omega_k t} - \frac{h_k}{\omega_k}b_k e^{-\mathrm{i}\omega_k t}\right)} U U^\dagger \sigma^+ U\rho_0\right\}\\
&= e^{+2\mathrm{i}\Omega t}\mathrm{Tr}\left\{e^{2\sum_k\left(\frac{h_k^*}{\omega_k}(b_k^\dagger + \frac{h_k}{\omega_k}\sigma^z)e^{+\mathrm{i}\omega_k t} - \frac{h_k}{\omega_k}(b_k + \frac{h_k^*}{\omega_k}\sigma^z)e^{-\mathrm{i}\omega_k t}\right)} e^{-2\sum_k\left(\frac{h_k^*}{\omega_k}b_k^\dagger - \frac{h_k}{\omega_k}b_k\right)}\sigma^+\rho_0\right\}\\
&= e^{+2\mathrm{i}\Omega t}\mathrm{Tr}\left\{e^{4\mathrm{i}\sum_k \frac{|h_k|^2}{\omega_k^2}\sin(\omega_k t)\sigma^z}\sigma^+\rho_S^0\right\}\mathrm{Tr}\left\{e^{2\sum_k\left(\frac{h_k^*}{\omega_k}b_k^\dagger e^{+\mathrm{i}\omega_k t} - \frac{h_k}{\omega_k}b_k e^{-\mathrm{i}\omega_k t}\right)} e^{-2\sum_k\left(\frac{h_k^*}{\omega_k}b_k^\dagger - \frac{h_k}{\omega_k}b_k\right)}\bar\rho_B\right\}\\
&= e^{+2\mathrm{i}\Omega t}\mathrm{Tr}\left\{e^{4\mathrm{i}\sum_k \frac{|h_k|^2}{\omega_k^2}\sin(\omega_k t)\sigma^z}\sigma^+\rho_S^0\right\} B(t)\,,
\end{aligned}
\tag{4.6}
$$

where we have used initial factorization $\rho_0 = \rho_S^0 \otimes \bar\rho_B$. Using that $e^X e^Y = e^{X+Y+[X,Y]/2}$ when $[X,[X,Y]] = [Y,[X,Y]] = 0$, we can further evaluate the decoherence factor resulting from the reservoir

$$
\begin{aligned}
B(t) &= \mathrm{Tr}\left\{\exp\left\{2\sum_k\left[\frac{h_k^*}{\omega_k}b_k^\dagger\left(e^{+\mathrm{i}\omega_k t}-1\right) - \frac{h_k}{\omega_k}b_k\left(e^{-\mathrm{i}\omega_k t}-1\right)\right]\right\}\bar\rho_B\right\} e^{-4\mathrm{i}\sum_k \frac{|h_k|^2}{\omega_k^2}\sin(\omega_k t)}\\
&= \mathrm{Tr}\left\{\exp\left\{+2\sum_k \frac{h_k^*}{\omega_k}b_k^\dagger\left(e^{+\mathrm{i}\omega_k t}-1\right)\right\}\exp\left\{-2\sum_k\frac{h_k}{\omega_k}b_k\left(e^{-\mathrm{i}\omega_k t}-1\right)\right\}\bar\rho_B\right\}\times\\
&\quad\times e^{-4\sum_k \frac{|h_k|^2}{\omega_k^2}[1-\cos(\omega_k t)+\mathrm{i}\sin(\omega_k t)]}\,.
\end{aligned}
\tag{4.7}
$$

Now, we can use that

$$
\begin{aligned}
\mathrm{Tr}\left\{e^{+\alpha_k b_k^\dagger}e^{-\alpha_k^* b_k}\frac{e^{-\beta\omega_k b_k^\dagger b_k}}{Z_k}\right\} &= \sum_{n,m=0}^\infty \frac{(+\alpha_k)^n(-\alpha_k^*)^m}{n!m!}\mathrm{Tr}\left\{(b_k^\dagger)^n b_k^m \frac{e^{-\beta\omega_k b_k^\dagger b_k}}{Z_k}\right\}\\
&= \sum_{q=0}^\infty\sum_{n=0}^q \frac{(-|\alpha_k|^2)^n}{(n!)^2}(1-e^{-\beta\omega_k})e^{-\beta\omega_k q}\frac{q!}{(q-n)!}\\
&= e^{-|\alpha_k|^2 n_B(\omega_k)}
\end{aligned}
\tag{4.8}
$$

with $|\alpha_k|^2 = 8|h_k|^2/\omega_k^2[1-\cos(\omega_k t)]$. This then implies for the decoherence factor

$$
B(t) = \exp\left\{-\frac{2}{\pi}\int_0^\infty \frac{\Gamma(\omega)}{\omega^2}[1-\cos(\omega t)][1+2n_B(\omega)]d\omega\right\}\exp\left\{-\frac{2\mathrm{i}}{\pi}\int_0^\infty\frac{\Gamma(\omega)}{\omega^2}\sin(\omega t)d\omega\right\}\,. \tag{4.9}
$$

Eventually, it follows that the populations remain unaffected and that in the interaction picture the coherences decay according to [2]

$$
\begin{aligned}
\boldsymbol{\rho_{01}}(t) &= \exp\left\{-8\sum_k |h_k|^2\frac{\sin^2(\omega_k t/2)}{\omega_k^2}\coth\left(\frac{\beta\omega_k}{2}\right)\right\}\rho_{01}^0\\
&= \exp\left\{-\frac{4}{\pi}\int_0^\infty \Gamma(\omega)\frac{\sin^2(\omega t/2)}{\omega^2}\coth\left(\frac{\beta\omega}{2}\right)d\omega\right\}\rho_{01}^0\,.
\end{aligned}
\tag{4.10}
$$

This result holds in a similar fashion also for multiple qubits as long as all the interactions do mutually commute [3]. For later comparison, we note that the above solution is also the solution of the **exact master equation**

$$\dot{\boldsymbol{\rho}} = +\frac{\dot{f}(t)}{2}\left(\sigma^z \boldsymbol{\rho} \sigma^z - \boldsymbol{\rho}\right)\,, \qquad f(t) = \frac{4}{\pi}\int_0^\infty \Gamma(\omega)\frac{\sin^2\left(\frac{\omega t}{2}\right)}{\omega^2}\coth\left(\frac{\beta\omega}{2}\right) d\omega\,, \tag{4.11}$$

and that $\dot{f} < 0$ may occur for specific times, depending on the specific form of $\Gamma(\omega)$. This shows that exact dynamics is not necessarily of Lindblad form. By using that

$$\lim_{t\to\infty} t\mathrm{sinc}^2\left(\frac{\omega t}{2}\right) = 2\pi\delta(\omega) \tag{4.12}$$

we can infer that $\lim\limits_{t\to\infty} f(t) = t\lim_{\omega\to 0}\Gamma(\omega)[1+2n_B(\omega)]$, such that the Markovian Lindblad master equation becomes in the long run $\dot{\boldsymbol{\rho}} = \lim_{\omega\to 0}\Gamma(\omega)[1+2n_B(\omega)]\left(\sigma^z\boldsymbol{\rho}\sigma^z - \boldsymbol{\rho}\right)$.

Using the polaron transform, we can also compute

$$\begin{aligned}
\left\langle b_k^\dagger b_k\right\rangle_t &= \mathrm{Tr}\left\{e^{+\mathrm{i}Ht} b_k^\dagger b_k e^{-\mathrm{i}Ht}\rho_0\right\} \\
&= \mathrm{Tr}\left\{U^\dagger e^{+\mathrm{i}\Omega t\sigma^z} e^{+\mathrm{i}\sum_k \omega_k t b_k^\dagger b_k} U b_k^\dagger b_k U^\dagger e^{-\mathrm{i}\Omega t\sigma^z} e^{-\mathrm{i}\sum_k \omega_k t b_k^\dagger b_k} U\rho_0\right\} \\
&= \mathrm{Tr}\left\{U^\dagger \left[b_k^\dagger e^{+\mathrm{i}\omega_k t} - \frac{h_k}{\omega_k}\sigma^z\right]\left[b_k e^{-\mathrm{i}\omega_k t} - \frac{h_k^*}{\omega_k}\sigma^z\right] U\rho_0\right\} \\
&= \mathrm{Tr}\left\{\left[\left(b_k^\dagger + \frac{h_k}{\omega_k}\right)e^{+\mathrm{i}\omega_k t} - \frac{h_k}{\omega_k}\sigma^z\right]\left[\left(b_k + \frac{h_k^*}{\omega_k}\right)e^{-\mathrm{i}\omega_k t} - \frac{h_k^*}{\omega_k}\sigma^z\right]\rho_0\right\} \\
&= \left\langle b_k^\dagger b_k\right\rangle_0 + \frac{\left|h_k\right|^2}{\omega_k^2} 2[1-\cos(\omega_k t)]\,,
\end{aligned} \tag{4.13}$$

where in the first line we used the polaron transform U, then performed successively all the unitary transformations in the middle, and eventually performed the inverse polaron transform (corresponding to $h_k \to -h_k$). From the above, we can conclude that the change of the reservoir energy becomes This already tells us that the total expectation value of the reservoir energy becomes

$$\Delta E(t) = \sum_k \omega_k \left\langle b_k^\dagger b_k\right\rangle_t - \sum_k \omega_k\left\langle b_k^\dagger b_k\right\rangle_0 = \frac{2}{\pi}\int_0^\infty \frac{\Gamma(\omega)}{\omega}\sin^2\left(\frac{\omega t}{2}\right) d\omega\,, \tag{4.14}$$

which is always positive.

In complete analogy one can compute the change of the reservoir particle number

$$\Delta N(t) = \frac{2}{\pi}\int_0^\infty \frac{J(\omega)}{\omega^2}\sin^2\left(\frac{\omega t}{2}\right) d\omega\,. \tag{4.15}$$

For a single reservoir, the exact solution for the total entropy production becomes

$$\Delta_{\mathrm{i}} S(t) = S(t) - S(0) + \beta\left[\Delta E(t) - \mu\Delta N(t)\right]\,. \tag{4.16}$$

Using that $\Delta E(t) > 0$, $\Delta N(t) > 0$, and for bosons $\mu \leq 0$ (actually, we would normally drop it for photons), we can already conclude that the second term that describes the reservoir entropy production is separately positive. Also, if we would let $t \to \infty$, the final density matrix of the system would be diagonal, such that we can conclude that $S(\infty) - S(0) > 0$, but does this hold for all times? Parametrizing the density matrix by the occupation ρ_{11} and the time-dependent coherence $\rho_{01}(t)$, its von-Neumann entropy becomes

$$\begin{aligned} S(t) = &-\frac{1}{2}\left[1 - \sqrt{(1-2\rho_{11})^2 + 4\left|\rho_{01}(t)\right|^2}\right] \ln \frac{1}{2}\left[1 - \sqrt{(1-2\rho_{11})^2 + 4\left|\rho_{01}(t)\right|^2}\right] \\ &-\frac{1}{2}\left[1 + \sqrt{(1-2\rho_{11})^2 + 4\left|\rho_{01}(t)\right|^2}\right] \ln \frac{1}{2}\left[1 + \sqrt{(1-2\rho_{11})^2 + 4\left|\rho_{01}(t)\right|^2}\right] . \end{aligned} \tag{4.17}$$

Using that as time increases, the coherences become smaller $\left|\rho_{01}(t)\right|^2 = e^{-2f(t)}\left|\rho_{01}^0\right|^2$, we find (in the regime $0 \le (1-2\rho_{11})^2 + 4\left|\rho_{01}(t)\right|^2 \le 1$ that is allowed for a valid density matrix), that $S(t) = -(1-x)/2 \ln(1-x)/2 - (1+x)/2 \ln(1+x)/2$ is a decaying function with $\sqrt{(1-2\rho_{11})^2 + 4\left|\rho_{01}(t)\right|^2} = x \in [0,1]$. Therefore, we conclude $S(t) > S(0)$, and consequently

$$\Delta_{\rm i} S(t) = S(t) - S(0) + \beta\left[\Delta E(t) - \mu \Delta N(t)\right] \ge 0 \,, \tag{4.18}$$

confirming the validity of the second law for the pure-dephasing model. Here, the first term gives the entropy increase in the system. The time derivative of these terms may become negative (similar to the discussion of the trace distance).

Bibliography

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[3] D. A. Lidar, Z. Bihary, and K. B. Whaley. From completely positive maps to the quantum Markovian semigroup master equation. *Chemical Physics*, 268:35–53, 2001.