DETAILED DERIVATION OF THE GENERAL MASTER EQUATION IN QUANTUM OPTICS

TIMOTHY JONES

Abstract. An unoriginal but more detailed derivation that typical is presented of the master equation.

1. Assumptions

We begin by outlining the assumptions which enable the canonical derivation of the master equation. Our general assumption is that our system is a harmonic oscillator $(aa\dagger)$ which interacts with a bath of oscillators $(\sum_i b_i b_i\dagger)$. Specifically:

1. We assume that the energy spectrum of the bath of oscillators is spaced tightly enough relative to its overall domain, i.e. $\omega_i \ll (\omega_N - \omega_0)$ such that the approximation $\sum_i \rightarrow \int d\omega_i g(\omega_i)$, where $g(\omega_i)$ is the density of states of the reservoir, is a physically acceptable mathematical assumption.

2. Related to the previous assumption, we assume that the bath is large enough and in a state of equilibrium such that any perturbations caused by the individual system on the bath is negligible. This is to say, the future state of the system-bath density operator is determined by its current state, and is not a function of the history of the bath (that is, we assume $\rho_{sb} = \rho_s(t) \otimes \rho_b(0)$). This is the Markoffian assumption.

3. We assume the rotating wave approximation regime. The interaction of the bath and system will have terms such as $ab, a\dagger b, ab\dagger, a\dagger b\dagger$. The lowering-lowering and raising-raising coupling has a much slower varying contribution to the state of the system, and so are excluded to give the interaction Hamiltonian $\sum_i g_i \left( a\dagger b_i + ab\dagger_i \right)$ where $g_i$ is a real coupling constant. Obviously, one must be certain the system one models can be simplified as such in order to apply the general master equation.

2. Construction of the Hamiltonian and Density Operators

We assume the system can be modeled with the Hamiltonian,

\begin{equation}
H_s = \hbar\omega a\dagger a, \quad [a, a\dagger] = 1
\end{equation}

Separately we assume that there exists a bath which can be modeled with the Hamiltonian,

\begin{equation}
H_b = \sum_i \hbar\omega_i b_i\dagger b_i, \quad [b_i, b_j\dagger] = \delta_{ik}
\end{equation}

Finally, as stated before, the interaction of the bath and system is taken in the form of

\begin{equation}
\sum_i g_i \left( a\dagger b_i + ab\dagger_i \right), \quad g_i \in \mathbb{R}
\end{equation}
The total Hamiltonian is,

\begin{equation}
H = \hbar \omega a^\dagger a + \sum_j \hbar \omega_j b_j^\dagger b_j + \sum_i g_i (a_i^\dagger b_i + a_i b_i^\dagger) + H_I
\end{equation}

We assume uncertainty in the preparation of states, so we switch to the density operator regime. We call the density operator corresponding to our bath coupled system \( \rho_{SB} \) (S: Single original oscillator; B: Environment) where the individual density operators can be retrieved via a trace, i.e.

\[ \rho_S = Tr_B(\rho_{SB}) = \sum_B \langle B | \rho_{SB} | B \rangle \] Trace over environment states

\[ \rho_B = Tr_S(\rho_{SB}) = \sum_S \langle S | \rho_{SB} | S \rangle \] Trace over local states

The dynamics of the system evolve as (Liouville equation),

\begin{equation}
i\hbar \frac{d\rho_{SE}}{dt} = [H, \rho_{SE}]\end{equation}

We commit a unitary transform to simplify this equation as follows (the so-called interaction picture). It can be shown that,

\begin{equation}
\exp(\alpha A)B\exp(-\alpha A) = B + \alpha [A, B] + \frac{\alpha^2}{2!} [A, [A, B]] + \cdots
\end{equation}

Furthermore, from the premises of Quantum Mechanics, it is legitimate to commit transforms of the type,

\begin{equation}
G' = \Lambda G \Lambda^\dagger, \quad \Lambda \in \text{Unitary}
\end{equation}

These so called similarity transformations preserve rank, determinant, trace, and eigenvalues. We let,

\begin{equation}
\rho_{se} = \exp \left( \frac{i}{\hbar} H_\circ t \right) \rho_{SE} \exp \left( - \frac{i}{\hbar} H_\circ t \right)
\end{equation}

We take the time derivative and find,

\begin{equation}
\frac{d\rho_{se}}{dt} = \frac{i}{\hbar} [H_\circ, \rho_{se}] - \frac{i}{\hbar} \exp \left( \frac{i}{\hbar} H_\circ t \right) [H, \rho_{SE}] \exp \left( - \frac{i}{\hbar} H_\circ t \right)
\end{equation}

From equation 2.6, since

\[ \Lambda G \Lambda^\dagger = \Lambda G^\dagger \Lambda H \Lambda^\dagger \]

and \([H_\circ, H_\circ] = 0\),

\[ \exp \left( \frac{i}{\hbar} H_\circ t \right) H_\circ \exp \left( - \frac{i}{\hbar} H_\circ t \right) = H_\circ \]

\begin{equation}
\frac{d\rho_{se}}{dt} = - \frac{i}{\hbar} [H_i, \rho_{se}]\end{equation}

where \(H_i\) is the transform of \(H_I\) and can be calculated as follows. We know that,

\[ [a^\dagger a, a^\dagger] = a^\dagger aa^\dagger - a^\dagger a^\dagger a = [a, a^\dagger] = a^\dagger \]

\[ [a^\dagger a, a] = a^\dagger aa - aa^\dagger a = [a^\dagger, a] = -a \]

and whereas \(H_\circ = \hbar \omega a^\dagger a\), equation 2.6 gives

\[ \exp(\alpha a^\dagger a) a^\dagger \exp(-\alpha a a^\dagger) = \exp(\alpha) a^\dagger, \]

\[ \exp(\alpha a a^\dagger) a \exp(-\alpha a^\dagger a) = \exp(-\alpha) a, \quad \alpha \in \mathbb{C} \]
\( H_i \) can be calculated in this fashion for both the \( aa^\dagger \) and the multiple set \( bb_i^\dagger \), where it is thus now trivial to find that,

\[
H_i(t) = \sum_i \hbar g_i \left( a_i^\dagger b_j \exp((i(\omega - \omega_i)t) + ab_i^\dagger \exp(-i(\omega - \omega_i)t) \right)
\]

If we now define

\[
G(t) = \sum_i g_i b_i \exp(i(\omega - \omega_j)t)
\]

we can simplify to

\[
H_i(t) = \hbar \left( G(t)a_i^\dagger + G^\dagger(t)a \right)
\]

Since the bath is in equilibrium, we can construct \( \rho_e(0) \) easily. Let \( Z_i = \exp(-\hbar \omega_i/kT) \). Then the probability that one mode (i) of the field is excited with n photons is

\[
P_{i,n} = \frac{Z_i^n}{\sum_n Z_i^n} = (1 - Z_i)Z_i^n = \left( 1 - \exp\left(\frac{-\hbar \omega_i}{kT}\right) \right) \exp\left(\frac{-n\hbar \omega_i}{kT}\right)
\]

The density matrix for this mode is then

\[
\rho_{e,i} = \left( 1 - \exp\left(\frac{-\hbar \omega_i}{kT}\right) \right) \sum_n \exp\left(\frac{-n\hbar \omega_i}{kT}\right) |n\rangle\langle n|
\]

To simplify this further, we imagine a three states system in which we can represent \( bb_i^\dagger |n\rangle = n |n\rangle \) as, for example letting \( n = 2 \),

\[
\begin{pmatrix}
0 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 2
\end{pmatrix}
\begin{pmatrix}
0 \\
0 \\
1
\end{pmatrix}
= 2
\begin{pmatrix}
0 \\
0 \\
1
\end{pmatrix}
\]

The above sum could then be written,

\[
0 \begin{pmatrix}
1 \\
0 \\
0
\end{pmatrix} \left[ 1 \ 0 \ 0 \right] + 1 \begin{pmatrix}
0 \\
1 \\
0
\end{pmatrix} \left[ 0 \ 1 \ 0 \right] + 2 \begin{pmatrix}
0 \\
0 \\
1
\end{pmatrix} \left[ 0 \ 0 \ 1 \right]
\]

We recover the matrix, and so we can write just as well,

\[
\rho_{e,i} = \left( 1 - \exp\left(\frac{-\hbar \omega_i}{kT}\right) \right) \exp\left(\frac{-b_i^\dagger b_i \hbar \omega_i}{kT}\right)
\]

By the rules of probability, the density operator for the entire bath becomes,

\[
\rho_e = \prod_i \left( 1 - \exp\left(\frac{-\hbar \omega_i}{kT}\right) \right) \exp\left(\frac{-b_i^\dagger b_i \hbar \omega_i}{kT}\right)
\]

By our assumptions, this is the state of the bath for all time, and so we will not write this as a function of time. The form \( \rho_e(t) \) will take will be much more complicated, and it is the purpose of this report to derive the differential equation defining its time evolution.
3. The Integration

Beginning with Equation 2.10, we take the first integration to get,

\[ \rho_{se}(t) = \rho_{se}(0) + \frac{1}{i\hbar} \int_0^t [H_i(t'), \rho_{se}(t')] dt' \]

(3.1)

Taking this result, we plug it into itself and get,

\[ \rho_{se}(t) = \rho_{se}(0) + \frac{1}{i\hbar} \int_0^t \int_0^{t'} [H_i(t'), [H_i(t''), \rho_{se}(t'')]] dt'' dt' \]

(3.2)

Quoting Narducci, “now we do something unexpected” and differentiate this equation. Since,

\[ \frac{d\rho_{se}}{dt}|_{t=0} = \frac{1}{i\hbar} [H_i(0), \rho_{se}(0)] \]

and

\[ \int_0^0 \text{anything} = 0 \]

we get the result,

\[ \frac{\rho_{se}(t)}{dt} = \frac{1}{i\hbar} [H_i(t), \rho_{se}(0)] - \frac{1}{\hbar^2} \int_0^t [H_i(t), [H_i(t'), \rho_{se}(t')]] \]

(3.3)

4. The Trace

To extract \( \rho_s \) we now need to trace over the environmental variables, i.e. average out the environmental degrees of freedom. We can most quickly see that,

\[ Tr_e[H_i(t), \rho_{se}] = 0 \]

(4.1)

as \( H_i \) is linear with \( b_j^l, \rho_{se} = \rho_s \rho_e \), and it is self evident that

\[ Tr_e b_j \exp(-\hbar \omega_j b_j^l/b_j^c/kT) = 0 \]

Thus we are left with,

\[ \frac{d\rho_s(t)}{dt} = \frac{1}{\hbar^2} \int_0^t Tr_e [H_i(t), [H_i(t'), \rho_{se}(t')]] \]

(4.2)

To proceed from here will require some care.

4.1. The partition. We first note that

\[ [H_i(t'), \rho_{se}(t')] = H_i(t')\rho_{se}(t') - \rho_{se}(t')H_i(t') \]

which we use to write \([H_i(t), [H_i(t'), \rho_{se}(t')]] =\)

\[ \frac{A}{H_i(t)H_i(t')\rho_{se}(t')} - \frac{B}{H_i(t)\rho_{se}(t')H_i(t')} - \frac{C}{H_i(t')\rho_{se}(t')H_i(t)} + \frac{D}{\rho_{se}(t')H_i(t')H_i(t)} \]

We will now proceed to treat the integration case by case.
4.2. Case A.

\[ H_i(t)H_i(t')\rho_{se}(t') = \]

\[ \hbar^2 (G(t)a^\dagger + G^i(t)a) (G(t')a^\dagger + G^i(t')a) \rho_s(t') \prod_i \left( 1 - \exp \left( \frac{-\hbar \omega_i}{kT} \right) \right) \exp \left( \frac{-b_j^\dagger b_j \hbar \omega_i}{kT} \right) \]

The first term we can extract is,

\[ \hbar^2 (G(t)a^\dagger G^i(t')a) \rho_s(t') \prod_i \left( 1 - \exp \left( \frac{-\hbar \omega_i}{kT} \right) \right) \exp \left( \frac{-b_j^\dagger b_j \hbar \omega_i}{kT} \right) \]

We recall that

\[ G(t) = \sum_j g_j b_j \exp(i(\omega - \omega_j)t) \]

so we can rewrite the term as (with \( \zeta = \hbar^2 a^\dagger a \rho_s(t') \) and \( \chi_i = \left[ 1 - \exp \left( \frac{-\hbar \omega_i}{kT} \right) \right] \)),

\[ \zeta \left[ \sum_j g_j^2 b_j^\dagger b_j \exp(i(\omega - \omega_j)(t - t')) \right] \prod_i \chi_i \exp \left( \frac{-b_j^\dagger b_j \hbar \omega_i}{kT} \right) \]

It is easily seen that when we take the trace, all terms will involve \( b_j b_j^\dagger \) and will vanish unless \( j = k \), so we can write the term as,

\[ \zeta \left[ \sum_j \chi_j g_j^2 b_j^\dagger b_j \exp(i(\omega - \omega_j)(t - t')) \right] \prod_i \chi_i \exp \left( \frac{-b_j^\dagger b_j \hbar \omega_i}{kT} \right) \]

But again, we can use the same argument to write the term as,

\[ \zeta \left[ \sum_j \chi_j g_j^2 b_j^\dagger b_j \exp(i(\omega - \omega_j)(t - t')) \right] \prod_i \chi_i \exp \left( \frac{-b_j^\dagger b_j \hbar \omega_i}{kT} \right) \]

We can now easily take the trace, noting that \( Tr[B\rho] = <B > \), and with \( n = b^\dagger b \) with \([b, b^\dagger] = 1 \).

\[ Tr \left\{ \zeta \sum_j \chi_j g_j^2 b_j^\dagger b_j \exp(i(\omega - \omega_j)(t - t')) \exp \left( \frac{-b_j^\dagger b_j \hbar \omega_i}{kT} \right) \right\} \]

\[ = \zeta \sum_j g_j^2 (1 + \bar{n}_j) \exp(i(\omega - \omega_j)(t - t')) \]

For the reader interested in the total details of the previous calculation, [1] is a good reference, where it is also demonstrated that, for example,

\[ \frac{\sum_0^\infty \langle n | b^\dagger b e^{-\lambda b^\dagger b} | n \rangle}{\sum_0^\infty \langle n | e^{-\lambda b^\dagger b} | n \rangle} = (1 - e^{-\lambda}) \sum_0^\infty ne^{-\lambda n} = \frac{1}{e^\lambda - 1} = \bar{n} \]

In any case, we now have a general formula we can use, that is,

\[ (G(t)G(t')) = (G^i(t)G^i(t')) = 0 \]

\[ (G(t)G^i(t')) = \sum_j (1 + \bar{n}_j) \exp(i(\omega - \omega_j)(t - t')) \]

\[ (G^i(t)G(t')) = \sum_j (\bar{n}_j) \exp(-i(\omega - \omega_j)(t - t')) \]

The other non zero trace will be, with \( \eta = \hbar^2 aa^\dagger \rho_s(t') \) and \( \gamma_j = \exp(i(\omega - \omega_j)(t - t')) \)

\[ Tr \left[ \eta (G(t)G(t')) \prod_i \chi_i \exp \left( \frac{-b_j^\dagger b_j \hbar \omega_i}{kT} \right) \right] = \eta \sum_j g_j^2 \bar{n}_j \gamma_j^\dagger \]
4.3. Case B.

\[ H(t) \rho_a(t') H(t') = \hbar^2 (G(t)a^\dagger + G^\dagger(t)a) \rho_a(t') (G(t')a^\dagger + G^\dagger(t')a) \]

Based on arguments of Case B, we consider, \( \alpha = \hbar^2a^\dagger \rho_a(t')a, \beta = \hbar^2a^\dagger \rho_a(t')a^\dagger, \)

\[
\hbar^2 a^\dagger \rho_a(t')a G(t) \rho_a G^\dagger(t') \rightarrow \alpha \text{Tr} \left\{ \sum_j \chi_j g^\dagger_j b_j \exp \left( -\frac{b_j h \omega_j}{kT} \right) b_j^\dagger \right\}
\]

\[
\hbar^2 \alpha a^\dagger \rho_a(t')a G^\dagger(t) \rho_a G(t') \rightarrow \beta \text{Tr} \left\{ \sum_j \chi_j g^\dagger_j b_j \exp \left( -\frac{b_j h \omega_j}{kT} \right) b_j^\dagger \right\}
\]

To these calculations we simply must note that,

\[
\langle n|b^\dagger b|n \rangle = (n + 1)(n + 1)|e^{-b^\dagger b}\rangle|n + 1\rangle
\]

Thus 4.3 becomes,

\[
(1 - e^{-\lambda}) e^{-\lambda} \sum_n (n + 1) e^{-\lambda n} = e^{-\lambda}(1 + \bar{n})
\]

We notice that,

\[
\frac{1}{e^{\lambda} - 1} = \bar{n} \rightarrow \frac{1 + \bar{n}}{\bar{n}} = e^\lambda, \quad \frac{\bar{n}}{1 + \bar{n}} = e^{-\lambda}
\]

\[
\hbar^2 \alpha a^\dagger \rho_a(t')a G(t) \rho_a G^\dagger(t') \rightarrow \alpha \sum_j g^\dagger_j \bar{n}_j \gamma_j
\]

\[
\hbar^2 \alpha a^\dagger \rho_a(t')a G^\dagger(t) \rho_a G(t') \rightarrow \beta \sum_j g^\dagger_j (1 + \bar{n}_j) \gamma_j^\dagger
\]

4.4. Case C.D. The remaining cases are easy to project from the two previous cases:

<table>
<thead>
<tr>
<th>Original Term</th>
<th>(1 + \bar{n}) result</th>
<th>(\bar{n}) result</th>
</tr>
</thead>
<tbody>
<tr>
<td>(H(t)H(t')\rho_a(t'))</td>
<td>(\hbar^2 a^\dagger \rho_a(t')a \sum_j g^\dagger_j (1 + \bar{n}_j) \gamma_j)</td>
<td>(\hbar^2 a a^\dagger \rho_a(t')a \sum_j g^\dagger_j \bar{n}_j \gamma_j)</td>
</tr>
<tr>
<td>(\rho_a(t')H(t')H(t))</td>
<td>(\hbar^2 \rho_a(t')a^\dagger a \sum_j g^\dagger_j (1 + \bar{n}_j) \gamma_j)</td>
<td>(\hbar^2 \rho_a(t')a a^\dagger \sum_j g^\dagger_j \bar{n}_j \gamma_j)</td>
</tr>
<tr>
<td>(\rho_a(t')H(t'H(t'))</td>
<td>(-\hbar^2 \rho_a(t')a^\dagger \sum_j g^\dagger_j (1 + \bar{n}_j) \gamma_j^\dagger)</td>
<td>(-\hbar^2 \rho_a(t')a \sum_j g^\dagger_j \bar{n}_j \gamma_j)</td>
</tr>
<tr>
<td>(-H(t')\rho_a(t'H(t))</td>
<td>(-\hbar^2 \rho_a(t')a^\dagger \sum_j g^\dagger_j (1 + \bar{n}_j) \gamma_j)</td>
<td>(-\hbar^2 \rho_a(t')a \sum_j g^\dagger_j \bar{n}_j \gamma_j)</td>
</tr>
</tbody>
</table>

5. The Summation Transform

In the approximation of the spectrum as continuous, we can use the transform,

\[
\sum_j \rightarrow \int d\omega_j D(\omega_j)
\]
6. Sokhotsky-Plemelj formula

The proper method of limiting this point to the real axis is to give the line of integration a small semi-circle bump below the real axis to accommodate the point. One then takes the radius of this semi-circle to zero and achieves the proper integral. It can be shown that the proper form of this integration is given by

\[ \lim_{y \downarrow 0} \int_{-\infty}^{\infty} \frac{f(x)}{x - x_0 - iy} dx = p.v. \int_{-\infty}^{\infty} \frac{f(x)}{x - x_0} dx + \lim_{y \downarrow 0} \int_{S} \frac{f(\eta)}{\eta - x_0} d\eta \]

The latter is taken over a semicircle which can be shrunk in the limit and thus equals \( \pi i f(x_0) \). Using the postulate of the Dirac delta function, we can write,

\[ \lim_{y \downarrow 0} \int_{-\infty}^{\infty} \frac{f(x)}{x - x_0 - iy} dx = p.v. \int_{-\infty}^{\infty} \frac{f(x)}{x - x_0} dx + i \pi \int_{-\infty}^{\infty} \delta(x - x_0)f(x) dx \]

This is typically approximated in theoretical physics as,

\[ \lim_{y \downarrow 0} \int_{-\infty}^{\infty} \frac{f(x)}{x - x_0 - iy} dx = p.v. \int_{-\infty}^{\infty} \frac{f(x)}{x - x_0} dx + \frac{i \pi}{x - x_0} + \int_{-\infty}^{\infty} \delta(x - x_0)f(x) dx \]

We note that, with \( \tau = t - t' \), \( d\tau = -dt' \),

\[ -\int_{0}^{t} \exp(i(\omega - \omega_j)\tau) d\tau = \left( \frac{i}{\omega - \omega_j} \right) [1 - \exp(i(\omega - \omega_j)t)] \]

The exponential term approximately averages out over the \( \omega \) integration, and we have the approximation,

\[ \int_{0}^{t} dt' e^{i(\omega - \omega_j)(t-t')} = \pi \delta(\omega - \omega_j) \pm iP\left( \frac{1}{\omega - \omega_j} \right) \]

Now looking at the table of calculations on the previous page, we see that many principal value part terms will cancel out, specifically, the B and C terms (i.e. \( \gamma \) cancels \( \gamma^\dagger \) whenever all other terms are equal).

For the A D terms, we must do something fancy, that is, use that \( aa^\dagger = 1 + a^\dagger a \) to convert all terms to \( a^\dagger a \) terms. This will create terms with \( a \) operators, but we notice the symmetry between these terms and that they cancel. We also see the antisymmetry across each row for the A and D terms, but since \( 1 + \bar{n} - \bar{n} = 1 \), we are left with only one set of terms which retain their principal value part.

We could articulate these details, but we feel that it will profit the reader to examine this by the table presented in this report.

The Dirac delta function will act as we would expect and drop out the \( \omega_j \) terms to \( \omega \), and so we will have our final terms.

7. Result

Once we finally take account of all terms, we find that, with \( \epsilon = \pi g(\omega)^2 D(\omega) \), and

\[ \Delta \omega = P \int_{0}^{\infty} \frac{g(\omega)^2 D(\omega)}{\omega - \omega_j} d\omega_j \]

\[ \frac{d\rho_s}{dt} = -i \Delta \omega [a^\dagger a, \rho_s(t)] - \epsilon(1 + \bar{n}) (\rho_s(t)a^\dagger a + a^\dagger a\rho_s(t) - 2a\rho_s(t)a^\dagger) \]

\[ -\epsilon(\bar{n}) (\rho_s(t)aa^\dagger + aa^\dagger \rho_s(t) - 2a^\dagger \rho_s(t)a) \]
REFERENCES

