PHYS 414: Mastering the master equation

The master equation has various forms and many implications. This write-up summarizes the ones we have seen so far in class.

1. Master equation in terms of the W matrix

The original form is a time evolution equation for the probability $p_m(t)$ of being in state m at time t, defined over an ensemble which has a distribution of states $p_n(0)$ at time zero:

$$\frac{dp_m}{dt} = \underbrace{\sum_{m'} W_{mm'} p_{m'}}_{\text{gain for state } m} - \underbrace{\sum_{m'} W_{m'm} p_m}_{\text{loss for state } m} . \tag{1}$$

The first sum on the right-hand side is the total probability flowing into state m, and the second one is the total probability flowing out. Note $W_{mn}\delta t$ is the probability of making a transition $n \to m$ over a small time interval δt, so $\sum_m W_{mn}\delta t = 1$. Thus each column of the W matrix (multiplied by δt) sums to 1. A *stationary distribution* p^s_m is defined by $dp^s_m/dt = 0$, so for p^s_m the gain is balanced by the loss.

2. Master equation in terms of the Ω matrix

Eq. (1) can be simplified by rewriting the right-hand side:

$$\begin{aligned}
\frac{dp_m}{dt} &= \sum_{m' \neq m} W_{mm'} p_{m'} + W_{mm} p_m - \sum_{m'} W_{m'm} p_m \\
&= \sum_{m' \neq m} W_{mm'} p_{m'} - \sum_{m' \neq m} W_{m'm} p_m \\
&= \sum_{m' \neq m} W_{mm'} p_{m'} + \left[- \sum_{\ell \neq m} W_{\ell m} \right] p_m \\
&= \sum_{m'} \Omega_{mm'} p_{m'},
\end{aligned} \tag{2}$$

where

$$\Omega_{mm'} \equiv \begin{cases} W_{mm'} & m \neq m' \\ -\sum_{\ell \neq m} W_{\ell m} & m = m' \end{cases} . \tag{3}$$

From the property $\delta t \sum_{m'} W_{m'm} = 1$ we see that $\sum_{m'} \Omega_{m'm} = 0$. Each column of the Ω matrix sums to zero.

The solution of the master equation for an arbitrary ensemble is:

$$p_m(t) = \sum_{m'} \left[e^{\Omega t} \right]_{mm'} p_{m'}(0), \tag{4}$$

where $\exp(\Omega t)$ is the matrix exponential of Ω. For a pure ensemble, where all copies are prepared in the same state n, $p_{m'}(0) = \delta_{m',n}$, and thus $p_m(t) = \left[e^{\Omega t} \right]_{mn} \equiv p_{mn}(t)$. So the individual components of the matrix exponential $P(t) \equiv \exp(\Omega t)$ correspond to pure ensemble probabilities $p_{mn}(t)$. The master equation can thus be written more compactly as

$$\frac{d\mathbf{p}}{dt} = \Omega\mathbf{p} \quad \text{or} \quad \frac{dP}{dt} = \Omega P. \tag{5}$$

Here $\mathbf{p}$ is a vector with components p_m. The difference between these two forms is that the first corresponds to an arbitrary ensemble, and the second one encompasses all possible pure ensembles. From Eq. (5) one can see that a stationary distribution $\mathbf{p}^s$ satisfying $d\mathbf{p}^s/dt = 0$ is a right eigenvector of Ω with eigenvalue zero: $\Omega\mathbf{p}^s = 0$. The second equation in Eq. (5), with the matrix components written out explicitly, gives us a master equation for the pure ensemble probabilities $p_{mn}(t)$:

$$\frac{dp_{mn}(t)}{dt} = \sum_{m'} \Omega_{mm'} p_{m'n}. \tag{6}$$

The initial conditions for this equation are $p_{mn}(0) = \delta_{m,n}$. Note that once you know the pure ensemble probabilities $p_{mn}(t) = [\exp(\Omega t)]_{mn}$, you can also calculate $p_m(t)$ for any arbitrary ensemble using $p_m(t) = \sum_n p_{mn}(t) p_n(0)$.

3. Adjoint master equation

Let us take the transpose of both sides of $dP/dt = \Omega P$. This gives $dP^T/dt = P^T\Omega^T$. In terms of individual components, the resulting equation is known as the adjoint master equation:

$$\frac{dp_{mn}}{dt} = \sum_{m'} p_{mm'} \Omega_{m'n}. \tag{7}$$

Using the definition of Ω from Eq. (3), this can also be rewritten in terms of the W matrix components:

$$\begin{aligned}
\frac{dp_{mn}}{dt} &= \sum_{m'} p_{mm'} \Omega_{m'n} \\
&= p_{mn}\Omega_{nn} + \sum_{m' \neq n} p_{mm'} \Omega_{m'n} \\
&= -p_{mn} \sum_{\ell \neq n} W_{\ell n} + \sum_{m' \neq n} p_{mm'} W_{m'n} \\
&= \sum_{m'} (p_{mm'} - p_{mn}) W_{m'n}.
\end{aligned} \tag{8}$$

The equality between the last two lines uses the fact that the $m' = n$ term in the sum in the last line equals zero. Thus there are two forms of the master equation for $p_{mn}(t)$, summarized here in both Ω and W versions:

$$\begin{aligned}
&\frac{dp_{mn}}{dt} = \sum_{m'} \Omega_{mm'} p_{m'n}, \qquad \frac{dp_{mn}}{dt} = \sum_{m'} \left[W_{mm'} p_{m'n} - W_{m'm} p_{mn}\right] \qquad \text{regular master equation} \\
&\frac{dp_{mn}}{dt} = \sum_{m'} p_{mm'} \Omega_{m'n}, \qquad \frac{dp_{mn}}{dt} = \sum_{m'} (p_{mm'} - p_{mn}) W_{m'n}. \qquad \text{adjoint master equation}
\end{aligned} \tag{9}$$

All of these are equivalent formulations, but some are more useful than others in various applications.

4. Survival probabilities and mean first passage times

One application of the adjoint master equation is in calculating the survival probability $U_{sn}(t)$, or the probability that if you start in state n at $t = 0$ (a pure ensemble), you have never visited state s in the time interval t. To calculate this probability, it is convenient to make the target state s a sink. In other words, set all the outgoing links W_{ms} which allow transitions out of s to zero. This way if you reach s, you will stay there. Assuming s is the only sink in the system (the simple case which we will consider here), and the network is connected, then the survival probability $U_{sn}(0) = 1$ and $U_{sn}(\infty) = 0$ for any $n \neq s$: the chances of survival are zero in the long time limit, since the system will eventually visit s. Similarly $U_{ss}(t) = 0$ for all t: if you start in s, by definition your survival probability is zero.

The survival probability $U_{sn}(t)$ can be related to the probabilities $p_{mn}(t)$ as follows:

$$U_{sn}(t) = \sum_{m \neq s} p_{mn}(t). \tag{10}$$

The probability of never having reached s by time t is just the sum over the probabilities of being in any state $m \neq s$ at time t. By taking the sum over $m \neq s$ of the adjoint master equation in Eq. (7), one finds an equation for $U_{sn}(t)$:

$$\frac{dU_{sn}}{dt} = \sum_{m'} U_{sm'} \Omega_{m'n} = \sum_{m' \neq s} U_{sm'} \Omega_{m'n}. \tag{11}$$

The second equality is due to $U_{ss} = 0$.

As time passes $U_{sn}(t)$ decreases, since at each moment there is some probability of the system reaching state s. The fraction of systems in the ensemble that reach s between t and $t + dt$ is given by $U_{sn}(t) - U_{sn}(t + dt) \approx dt(-dU_{sn}/dt) \equiv dt f_{sn}(t)$. The latter quantity $f_{sn}(t)$ is the *first passage time (FPT) distribution*, the probability per unit time of reaching s for the first time in the interval t to $t + dt$, assuming you started at n at time $t = 0$. The *mean first passage time (MFPT)* τ_{sn} is just the average time it takes to first reach s. Note that for $n = s$, $f_{ss}(t) = \delta(t)$ and $\tau_{sn} = 0$. If you are at s, the distribution of times to reach s is just a delta function at $t = 0$, and the mean time to reach s is zero.

In general τ_{sn} is an average over the FPT distribution,

$$\tau_{sn} = \int_0^\infty dt\, t f_{sn}(t) = -\int_0^\infty dt\, t \frac{dU_{sn}}{dt} = \int_0^\infty dt\, U_{sn}. \tag{12}$$

The last equality follows from integration by parts and the fact that $U_{sn}(\infty) = 0$. For $n \neq s$, let us integrate both sides of Eq. (11) over t from 0 to ∞, yielding the following equation:

$$\begin{aligned} U_{sn}(\infty) - U_{sn}(0) &= \sum_{m' \neq s} \tau_{sm'} \Omega_{m'n} \\ -1 &= \sum_{m' \neq s} \tau_{sm'} \Omega_{m'n} \end{aligned} \tag{13}$$

This equation, valid for all $n \neq s$, provides a way of recursively calculating any MFPT τ_{sn}.