The Large-Number Limit for Reaction Networks

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In John Baez's paper, **Quantum Techniques for Reaction Networks**, it was proved that

$$\frac{d}{dt}\langle N_i\psi(t)\rangle = \sum_{\tau\in T} r(\tau)(t_i(\tau) - s_i(\tau))\langle N^{\underline{s(\tau)}}\psi(t)\rangle.$$

Definition 1. *The* ***rescaled number operators*** *are defined as* $\widetilde{N}_i = \hbar N_i$.

Definition 2. *The* ***rescaled falling powers of number operators*** *are defined as*

$\widetilde{N}_i^{\underline{r_i}} = \widetilde{N}_i(\widetilde{N}_i - \hbar)(\widetilde{N}_i - 2\hbar)...(\widetilde{N}_i - r_i\hbar + \hbar)$ *for a specific index* i*, and*

$\widetilde{N}^{\underline{r}} = \widetilde{N}_1^{\underline{r_1}}\widetilde{N}_2^{\underline{r_2}}...\widetilde{N}_k^{\underline{r_k}}$ *for a multi index* r.

Using these, we get

$$\frac{1}{\hbar}\frac{d}{dt}\langle \widetilde{N}_i\psi(t)\rangle = \sum_{\tau\in T} r(\tau)(t_i(\tau) - s_i(\tau))\langle \widetilde{N}^{\underline{s(\tau)}}\psi(t)\rangle\frac{1}{\hbar^{|s(\tau)|}}$$

Definition 3. *The* ***rescaled rate constants*** *are* $\widetilde{r}(\tau) = \dfrac{r(\tau)}{\hbar^{|s(\tau)|-1}}$. *From now onwards, we consider the* $\widetilde{r}(\tau)$*s to be constant instead of the original* $r(\tau)$*s.*

Then, we get :

Definition 4. *the* ***rescaled master equation***, $\dfrac{d}{dt}\langle \widetilde{N}\widetilde{\psi}(t)\rangle = \displaystyle\sum_{\tau\in T}\widetilde{r}(\tau)(t(\tau) - s(\tau))\langle \widetilde{N}^{\underline{s(\tau)}}\widetilde{\psi}(t)\rangle$.
Here, $\langle \widetilde{N}\widetilde{\psi}(t)\rangle = (\langle \widetilde{N_1}\widetilde{\psi}(t)\rangle, \langle \widetilde{N_2}\widetilde{\psi}(t)\rangle, ...\langle \widetilde{N_k}\widetilde{\psi}(t)\rangle)$ *and*
$t(\tau) - s(\tau) = (t_1(\tau) - s_1(\tau), t_2(\tau) - s_2(\tau)...t_k(\tau) - s_k(\tau))$.

This is a one parameter family of equations, depending on $\hbar \in (0, \infty)$. *We represent a solution of this rescaled master equation by* $\widetilde{\psi}(t)$, *but it is really one solution for each value of* $\hbar$.

Following the same procedure as above, we can rescale the rate equation, using the same definition of the rescaled rate constants.

Definition 5. *The* ***rescaled number*** *of instances of the* i^{th} *species is defined as* $\widetilde{x}_i = \hbar x_i$, *where* x_i *is the original number of instances of the* i^{th} *species.*

We get

Definition 6. *the* ***rescaled rate equation****,* $\frac{d}{dt}\widetilde{x}(t) = \sum_{\tau \in T} \widetilde{r}(\tau)(t(\tau) - s(\tau))\widetilde{x}(t)^{s(\tau)}$, *where* $\widetilde{x}(t) = (\widetilde{x}_1(t), \widetilde{x}_2(t), \ldots.\widetilde{x}_k(t))$*.*

Therefore, to go from the rescaled master equation to the rescaled rate equation, we require

$\langle \widetilde{N}^{\underline{r}}\widetilde{\psi}(t)\rangle \to \langle \widetilde{N}^{r}\widetilde{\psi}(t)\rangle \to \langle \widetilde{N}\widetilde{\psi}(t)\rangle^{r}$ as $\hbar \to 0$.

Then we can identify $\langle \widetilde{N}\widetilde{\psi}(t)\rangle$ with $\widetilde{x}(t)$.

To this end, we introduce a new definition:

Definition 7. *A* ***semiclassical family of states****,* $\psi_\hbar$*, where* $\hbar \in (0, \infty)$*, is defined as the one parameter family of states, where*

for every $r \in \mathbb{N}^k$*, as* $\hbar \to 0$*,* $\langle \widetilde{N}^{r}\psi_\hbar\rangle \to \widetilde{c}^{r}$*, for some* $\widetilde{c} \in [0, \infty)^k$*.*

In particular, $\langle \widetilde{N}_i\psi_\hbar\rangle \to \widetilde{c}_i$ *for every index i.*

Proposition 1. *If* $\psi_\hbar$ *is a semiclassical family as defined above, then in the* $\hbar \to 0$ *limit, we have* $\langle \widetilde{N}^{\underline{r}}\psi_\hbar\rangle \to \widetilde{c}^{r}$ *as well.*

Proof. For each index i,

$\langle \widetilde{N}_i^{\underline{r}}\psi_\hbar\rangle = \langle (\widetilde{N}_i(\widetilde{N}_i - \hbar)(\widetilde{N}_i - 2\hbar)\ldots(\widetilde{N}_i - r\hbar + \hbar))\psi_\hbar\rangle$

$= \langle (\widetilde{N}_i^{r} + \hbar\frac{(r-1).r}{2}\widetilde{N}_i^{r-1} + \ldots.. + \hbar^{r-1}(r-1)!)\psi_\hbar\rangle$

Now, by the definition of a semiclassical family,

$$\lim_{\hbar \to 0}\langle (\widetilde{N}_i^{r} + \hbar\frac{(r-1).r}{2}\widetilde{N}_i^{r-1} + \ldots.. + \hbar^{r-1}(r-1)!)\psi_\hbar\rangle = \widetilde{c}_i^{r}$$

Therefore, $\langle \widetilde{N}^{\underline{r}}\psi_\hbar\rangle \to \widetilde{c}^{r}$, as $\hbar \to 0$.

□

Proposition 2. *If* $\psi_\hbar$ *is a semiclassical family of states, then the centred moments of* $\psi_\hbar$ *tend to 0 as* $\hbar \to 0$*.*

Proof. Consider the r_i^{th} moment of $\psi_\hbar$ for the index i, $\langle (\widetilde{N}_i - \widetilde{c}_i)^{r_i}\widetilde{\psi}_\hbar\rangle$.

Now, $\langle (\widetilde{N}_i - \widetilde{c}_i)^{r_i}\widetilde{\psi}_\hbar\rangle = \sum_{p=0}^{r_i}\binom{r_i}{p}\langle \widetilde{N}_i^{p}\widetilde{\psi}_\hbar\rangle(-\widetilde{c}_i)^{r_i-p}$

$$\therefore \lim_{\hbar \to 0}\sum_{p=0}^{r_i}\binom{r_i}{p}\langle \widetilde{N}_i^{p}\widetilde{\psi}_\hbar\rangle(-\widetilde{c}_i)^{r_i-p} \to \sum_{p=0}^{r_i}\binom{r_i}{p}(\widetilde{c}_i)^{p}(-\widetilde{c}_i)^{r_i-p} = (\widetilde{c}_i - \widetilde{c}_i)^{r_i} = 0.$$

For a general multi index r, $\langle (\widetilde{N}-\widetilde{c})^r \widetilde{\psi}_\hbar \rangle \to 0$ as $\hbar \to 0$.

$\square$

It is interesting to note that we could have defined a semiclassical family of states in terms of moments going to 0, as $\hbar \to 0$.

Proposition 3. *If for a state, $\psi_\hbar$, the centred moments tend to 0 as $\hbar \to 0$, then $\langle \widetilde{N}^r \psi_\hbar \rangle \to \widetilde{c}^r$, where c is the mean.*

Proof. Observe that $\langle (\widetilde{N}_i^{r_i} - \widetilde{c}_i^{r_i}) \widetilde{\psi}_\hbar \rangle = \displaystyle\sum_{k=1}^{r_i} \binom{r_i}{k} (\widetilde{c}_i)^{r_i-k} \langle (\widetilde{N}_i - \widetilde{c}_i)^k \widetilde{\psi}_\hbar \rangle$.

Therefore, if the moments tend to 0 as $\hbar \to 0$, we get $\langle \widetilde{N}_i^{r_i} \widetilde{\psi}_\hbar \rangle = \widetilde{c}_i^{r_i}$ and in general, $\langle \widetilde{N}^r \widetilde{\psi}_\hbar \rangle = \widetilde{c}^r$

$\square$

Theorem 1. *If $\widetilde{\psi}(t)$ is a solution of the rescaled master equation and also a semiclassical family for the time interval $[t_0, t_1]$, then*

$\widetilde{c}(t) = \langle \widetilde{N} \widetilde{\psi}(t) \rangle$ *is a solution of the rescaled rate equation for $t \in [t_o, t_1]$.*

An Example: Rescaled coherent states

Consider the family of coherent states, $\widetilde{\psi}_\hbar = \dfrac{e^{(\widetilde{c}/\hbar)z}}{e^{\widetilde{c}/\hbar}}$, using the notation developed in the earlier mentioned paper of John Baez.

In the same paper, it was shown that for any multi index m, and any coherent state Ψ, $\langle N^{\underline{m}} \Psi \rangle = \langle N \Psi \rangle^m$.

Using this result for $\widetilde{\psi}_\hbar$, we get

$$\langle \widetilde{N}^{\underline{m}} \widetilde{\psi}_\hbar \rangle \;=\; \hbar^{|m|} \langle \widetilde{N}^{\underline{m}} \widetilde{\psi}_\hbar \rangle \;=\; \hbar^{|m|} \langle N \widetilde{\psi}_\hbar \rangle^m \;=\; \hbar^{|m|} \frac{\widetilde{c}^m}{\hbar^{|m|}} \;=\; \widetilde{c}^m.$$

Note that $\widetilde{N}_i^{\underline{1}} = \widetilde{N}_i$ and $\langle \widetilde{N}_i^{\underline{1}} \widetilde{\psi}_\hbar \rangle = \widetilde{c}_i = \langle \widetilde{c}_i \psi_\hbar \rangle$.

So, for all powers p, $\langle (\widetilde{N}_i^{\underline{1}})^p \widetilde{\psi}_\hbar \rangle = \langle \widetilde{c}_i^{\,p} \psi_\hbar \rangle$.

Now, by definition, $\widetilde{N}_i^{\underline{m_i}} = \widetilde{N}_i (\widetilde{N}_i - \hbar) ... (\widetilde{N}_i - m_i \hbar + \hbar)$, and $\widetilde{N}_i = \widetilde{N}_i^{\underline{1}}$.

Therefore, as $\langle \widetilde{N}_i^{\underline{m_i}} \psi_\hbar \rangle = \langle ((\widetilde{N}_i^{\underline{1}})^{m_i} + \hbar \, \frac{(m_i-1).m_i}{2} \, (\widetilde{N}_i^{\underline{1}})^{m_i-1} + ... + \hbar^{m_i-1} (m_i-1)!) \psi_\hbar \rangle$

$= \langle (\widetilde{c}_i^{m_i} + \hbar \, \frac{(m_i-1).m_i}{2} \, \widetilde{c}_i^{m_i-1} + ... + \hbar^{m_i-1} (m_i-1)!) \psi_\hbar \rangle$

So, as $\hbar \to 0$, $\langle \widetilde{N}_i^{\underline{m_i}} \psi_\hbar \rangle \;\to\; \langle \widetilde{N}_i^{m_i} \psi_\hbar \rangle$.

In general, $\lim\limits_{\hbar \to 0} \langle \widetilde{N}^m \psi_\hbar \rangle \;=\; \widetilde{c}^m$, showing that our chosen $\psi_\hbar$ is indeed a semiclassical family.

Intuitively, it can be seen that our definition of a semiclassical family implies that the original probability distribution be sharply peaked with a very large mean.