CPMG Equations

Introduction

The general case for two-site exchange is:

$$R_2 = R_{2max} + \frac{1}{2}k_{ex} - \frac{1}{2\tau}cosh^{-1}\left(D_+cosh(\tau\lambda_+) - D_-cos(\tau\lambda_-)\right)$$

Here

$$\begin{aligned}
D_\pm &= \frac{1}{2}\left(\pm 1 + \frac{\Psi + 2\Delta\omega^2}{(\Psi^2+\zeta^2)^{1/2}}\right) \\
\lambda_\pm &= \frac{1}{\sqrt{2}}\left(\pm\Psi + (\Psi^2+\zeta^2)^{1/2}\right)^{1/2} \\
\Psi &= k_{ex}^2 - \Delta\omega^2 \\
\zeta &= 2\Delta\omega(k_{AB} - k_{BA}) \\
k_{ex} &= k_{AB} + k_{BA}
\end{aligned}$$

We also sometimes use $\nu = \frac{1}{2\tau}$ instead of τ.

Experimentally one measures R_2 for various τ and one wants to find R_{2max}, k_{AB}, k_{BA} and $\Delta\omega$ which give the best fit.

Case: $\tau \to 0$

Consider $\tau \to 0$ (or equivalently $\nu \to \infty$).

For small z we have that $cosh(z) \simeq 1 + \frac{1}{2}z^2$ and $cos(z) \simeq 1 - \frac{1}{2}z^2$. Thus we see that for small τ we have

Then

$$\begin{aligned}
cosh(\tau\lambda_+) &\simeq 1 + \frac{1}{2}\tau^2\lambda_+^2 \\
cos(\tau\lambda_-) &\simeq 1 - \frac{1}{2}\tau^2\lambda_-^2
\end{aligned}$$

Thus

$$\begin{aligned}
D_+cosh(\tau\lambda_+) - D_-cos(\tau\lambda_-) &\simeq D_+ - D_- + \frac{1}{2}\tau^2(D_+\lambda_+^2 + D_-\lambda_-^2) \\
&= 1 + \frac{1}{2}\tau^2(D_+\lambda_+^2 + D_-\lambda_-^2)
\end{aligned}$$

For small z we have that $cosh^{-1}(1+\frac{1}{2}z^2) \simeq z$. Therefore we see that for small τ we have

$$R_2 \simeq R_{2max} + \frac{1}{2}k_{ex} - \frac{1}{2}\left(D_+\lambda_+^2 + D_-\lambda_-^2\right)^{1/2}$$

Case: $\tau \to \infty$

Consider $\tau \to \infty$ (or equivalently $\nu \to 0$).

Then we can ignore the cosine term. For large z we have that $cosh(z) \simeq \frac{1}{2}e^z$. Thus we see that for large τ we have

$$D_+cosh(\tau\lambda_+) \simeq \frac{1}{2}D_+e^{\tau\lambda_+} = \frac{1}{2}e^{\tau\lambda_+ + lnD_+}$$

For large z we have that $cosh^{-1}(\frac{1}{2}e^z) \simeq z$. Therefore we see that for large τ we have

$$\begin{aligned} R_2 &\simeq R_{2max} + \frac{1}{2}k_{ex} - \frac{1}{2\tau}(\tau\lambda_+ + lnD_+) \\ &\simeq R_{2max} + \frac{1}{2}k_{ex} - \frac{1}{2}\lambda_+ \end{aligned}$$

Case: $k_{AB} = k_{BA}, \Psi > 0$

The assumption that $k_{AB} = k_{BA}$ makes the equations much simpler. Immediately we have $\zeta = 0$.

$\Psi > 0$ means that $k_{ex} > \Delta\omega$. With $\Psi > 0$ we also have

$$\begin{aligned} D_+ &= 1 + \frac{\Delta\omega^2}{\Psi} = \frac{k_{ex}^2}{\Psi} \\ D_- &= \frac{\Delta\omega^2}{\Psi} \\ \lambda_+ &= \Psi^{1/2} \\ \lambda_- &= 0 \end{aligned}$$

As $\tau \to 0$ we find that

$$
\begin{aligned}
R_2 &\simeq R_{2max} + \frac{1}{2}k_{ex} - \frac{1}{2}\left(D_+\lambda_+^2 + D_-\lambda_-^2\right)^{1/2} \\
&= R_{2max} + \frac{1}{2}k_{ex} - \frac{1}{2}D_+^{1/2}\lambda_+ \\
&= R_{2max} + \frac{1}{2}k_{ex} - \frac{1}{2}\frac{k_{ex}}{\Psi^{1/2}}\Psi^{1/2} \\
&= R_{2max}
\end{aligned}
$$

Thus looking at the smallest τ (largest ν) should determine a reasonable first estimate of R_{2max}.

As $\tau \to \infty$ we have that

$$
\begin{aligned}
R_2 &\simeq R_{2max} + \frac{1}{2}k_{ex} - \frac{1}{2}\lambda_+ \\
&= R_{2max} + \frac{1}{2}k_{ex} - \frac{1}{2}\Psi^{1/2} \\
&= R_{2max} + \frac{1}{2}k_{ex} - \frac{1}{2}(k_{ex}^2 - \Delta\omega^2)^{1/2}
\end{aligned}
$$

This doesn't help too much.

Case: $k_{AB} = k_{BA}, k_{ex} \gg \Delta\omega$

Fast exchange has $k_{ex} \gg \Delta\omega$, and this implies that $\Psi > 0$. We write

$$\Psi = k_{ex}^2 - \Delta\omega^2 = k_{ex}^2(1-\epsilon)$$

where $\epsilon = \frac{\Delta\omega^2}{k_{ex}^2} \ll 1$ and so is small.

Then to first order we have

$$\Psi^{1/2} = k_{ex}(1-\epsilon)^{1/2} \simeq k_{ex}(1 - \frac{1}{2}\epsilon)$$

and

$$\frac{1}{\Psi} = \frac{1}{k_{ex}^2}\frac{1}{(1-\epsilon)} \simeq \frac{1}{k_{ex}^2}(1+\epsilon)$$

Then

$$
\begin{aligned}
D_+ &= \frac{k_{ex}^2}{\Psi} \simeq 1 + \epsilon \\
D_- &= \frac{\Delta\omega^2}{\Psi} \simeq \epsilon \\
\lambda_+ &= \Psi^{1/2} \simeq k_{ex}(1 - \frac{1}{2}\epsilon) \\
\lambda_- &= 0
\end{aligned}
$$

It turns out to be easier not to expand λ_+ in terms of ϵ immediately but only later. Then

$$
\begin{aligned}
D_+cosh(\tau\lambda_+) - D_-cos(\tau\lambda_-) &\simeq (1+\epsilon)cosh(\tau\lambda_+) - \epsilon \\
&= cosh(\tau\lambda_+) + \epsilon\ (cosh(\tau\lambda_+) - 1) \\
&= A + B\epsilon
\end{aligned}
$$

where

$$
\begin{aligned}
A &= cosh(\tau\lambda_+) \\
B &= cosh(\tau\lambda_+) - 1
\end{aligned}
$$

We need to find $cosh^{-1}(A + B\epsilon) = C + D\epsilon$. Taking $cosh$ on both sides gives

$$
\begin{aligned}
A + B\epsilon &= cosh(C + D\epsilon) \\
&= cosh(C)cosh(D\epsilon) + sinh(C)sinh(D\epsilon) \\
&\simeq cosh(C) + D\epsilon\ sinh(C)
\end{aligned}
$$

and thus we have $A = cosh(C)$ and $B = D\ sinh(C)$ and so as long as $A \neq 1$ (as here except in special case $\tau = 0$) we have

$$
\begin{aligned}
C &= cosh^{-1}(A) \\
D &= \frac{B}{\sqrt{A^2 - 1}}
\end{aligned}
$$

Here that gives

$$
\begin{aligned}
C &= \tau\lambda_+ \\
D &= \frac{cosh(\tau\lambda_+) - 1}{\sqrt{cosh^2(\tau\lambda_+) - 1}} \\
&= \left(\frac{cosh(\tau\lambda_+) - 1}{cosh(\tau\lambda_+) + 1}\right)^{1/2} \\
&= tanh(\frac{1}{2}\tau\lambda_+)
\end{aligned}
$$

(from a standard half-angle formula). Therefore

$$\begin{aligned}
R_2 &\simeq R_{2max} + \frac{1}{2}k_{ex} - \frac{1}{2\tau}\left(\tau\lambda_+ + \epsilon\ tanh(\frac{1}{2}\tau\lambda_+)\right) \\
&\simeq R_{2max} + \frac{1}{2}k_{ex} - \frac{1}{2}\left(k_{ex}(1-\frac{1}{2}\epsilon) + \frac{\epsilon}{\tau}\ tanh(\frac{1}{2}\tau k_{ex})\right) \\
&= R_{2max} + \frac{\epsilon k_{ex}}{4}\left(1 - \frac{2}{\tau k_{ex}}tanh(\frac{1}{2}\tau k_{ex})\right) \\
&= R_{2max} + \frac{\Delta\omega^2}{4k_{ex}}\left(1 - \frac{2}{\tau k_{ex}}tanh(\frac{1}{2}\tau k_{ex})\right) \\
&= R_{2max} + \frac{\Delta\omega^2}{4k_{ex}}\left(1 - \frac{4\nu}{k_{ex}}tanh(\frac{k_{ex}}{4\nu})\right)
\end{aligned}$$

As before, in the limit as $\tau \to 0$ we have $R_2 \simeq R_{2max}$. The limit $\tau \to \infty$ gives

$$R_2 \simeq R_{2max} + \frac{\Delta\omega^2}{4k_{ex}}$$

Case: $k_{AB} = k_{BA}, \Psi < 0$

The assumption that $k_{AB} = k_{BA}$ makes the equations much simpler. Immediately we have $\zeta = 0$.

$\Psi < 0$ means that $k_{ex} < \Delta\omega$. With $\Psi < 0$ we also have

$$\begin{aligned}
D_+ &= \frac{\Delta\omega^2}{|\Psi|} \\
D_- &= -1 + \frac{\Delta\omega^2}{|\Psi|} = \frac{k_{ex}^2}{|\Psi|} \\
\lambda_+ &= 0 \\
\lambda_- &= |\Psi|^{1/2}
\end{aligned}$$

As $\tau \to 0$ we find that

$$\begin{aligned}
R_2 &\simeq R_{2max} + \frac{1}{2}k_{ex} - \frac{1}{2}\left(D_+\lambda_+^2 + D_-\lambda_-^2\right)^{1/2} \\
&= R_{2max} + \frac{1}{2}k_{ex} - \frac{1}{2}D_-^{1/2}\lambda_- \\
&= R_{2max} + \frac{1}{2}k_{ex} - \frac{1}{2}\frac{k_{ex}}{|\Psi|^{1/2}}|\Psi|^{1/2} \\
&= R_{2max}
\end{aligned}$$

This is the same result as for $\Psi > 0$, so again we can use the smallest τ (largest ν) to determine a reasonable first estimate of R_{2max}.

As $\tau \to \infty$ we have that

$$\begin{aligned} R_2 &\simeq R_{2max} + \frac{1}{2}k_{ex} - \frac{1}{2}\lambda_+ \\ &= R_{2max} + \frac{1}{2}k_{ex} \end{aligned}$$

Combined with the $\tau \to 0$ estimate of R_{2max} we see that we can use the largest τ (smallest ν) to determine a reasonable first estimate of k_{ex}.

Case: $k_{AB} = k_{BA}, k_{ex} \ll \Delta\omega$

Slow exchange has $k_{ex} \ll \Delta\omega$, and this implies that $\Psi < 0$. We write

$$\Psi = k_{ex}^2 - \Delta\omega^2 = -\Delta\omega^2(1 - \epsilon)$$

where $\epsilon = \frac{k_{ex}^2}{\Delta\omega^2} \ll 1$ and so is small.

Then to first order we have

$$|\Psi|^{1/2} = \Delta\omega(1 - \epsilon)^{1/2} \simeq \Delta\omega(1 - \frac{1}{2}\epsilon)$$

and

$$\frac{1}{|\Psi|} = \frac{1}{\Delta\omega^2}\frac{1}{(1 - \epsilon)} \simeq \frac{1}{\Delta\omega^2}(1 + \epsilon)$$

Then

$$\begin{aligned} D_+ &= \frac{\Delta\omega^2}{|\Psi|} \simeq 1 + \epsilon \\ D_- &= \frac{k_{ex}^2}{|\Psi|} \simeq \epsilon \\ \lambda_+ &= 0 \\ \lambda_- &= |\Psi|^{1/2} \simeq \Delta\omega(1 - \frac{1}{2}\epsilon) \simeq \Delta\omega \end{aligned}$$

It turns out to be easier not to expand λ_- in terms of ϵ. Then

$$\begin{aligned} D_+ cosh(\tau\lambda_+) - D_- cos(\tau\lambda_-) &\simeq (1+\epsilon) - \epsilon\ cos(\tau\lambda_-) \\ &= 1 + \epsilon\ (1 - cos(\tau\lambda_-)) \end{aligned}$$

For z small we have $cosh(z) \simeq 1 + \frac{1}{2}z^2$ and so we see that for small t we have $cosh^{-1}(1+t) \simeq (2t)^{1/2}$. Thus we have

$$\begin{aligned} R_2 &\simeq R_{2max} + \frac{1}{2}k_{ex} - \frac{1}{2\tau}\left(2\epsilon(1 - cos(\tau\lambda_-))\right)^{1/2} \\ &= R_{2max} + \frac{1}{2}k_{ex} - \frac{1}{2\tau}\left(4\epsilon\ sin^2(\frac{1}{2}\tau\lambda_-)\right)^{1/2} \\ &= R_{2max} + \frac{1}{2}k_{ex} - \frac{\epsilon^{1/2}}{\tau} sin(\frac{1}{2}\tau\lambda_-) \\ &\simeq R_{2max} + \frac{1}{2}k_{ex}\left(1 - \frac{2}{\tau\Delta\omega} sin(\frac{1}{2}\tau\Delta\omega)\right) \\ &= R_{2max} + \frac{1}{2}k_{ex}\left(1 - \frac{4\nu}{\Delta\omega} sin(\frac{\Delta\omega}{4\nu})\right) \end{aligned}$$

(using a standard half-angle formula).

Case: $k_{AB} = k_{BA}, k_{ex} \approx \Delta\omega$

The case when $k_{ex} \approx \Delta\omega$ is interesting because the general equation has singularities (which cancel) so making it numerically unsuitable. This does not happen if $k_{AB} \neq k_{BA}$ so that $\zeta \neq 0$.

First consider the case when $\Psi > 0$, so that $\epsilon = \Psi = k_{ex}^2 - \Delta\omega^2 > 0$ but is small. Then

$$\begin{aligned} D_+ &= 1 + \frac{\Delta\omega^2}{\Psi} = \frac{k_{ex}^2}{\epsilon} \\ D_- &= \frac{\Delta\omega^2}{\epsilon} \\ \lambda_+ &= \Psi^{1/2} = \epsilon^{1/2} \\ \lambda_- &= 0 \end{aligned}$$

Thus

$$\begin{aligned} D_+ cosh(\tau\lambda_+) - D_- cos(\tau\lambda_-) &= \frac{k_{ex}^2}{\epsilon} cosh(\tau\epsilon^{1/2}) - \frac{\Delta\omega^2}{\epsilon} \\ &\simeq \frac{1}{\epsilon}(k_{ex}^2(1 + \frac{1}{2}\tau^2\epsilon) - (k_{ex}^2 - \epsilon)) \\ &= 1 + \frac{1}{2}k_{ex}^2\tau^2 \end{aligned}$$

Therefore

$$R_2 \simeq R_{2max} + \frac{1}{2}k_{ex} - \frac{1}{2\tau}cosh^{-1}(1 + \frac{1}{2}k_{ex}^2\tau^2)$$

Next consider the case when $\Psi < 0$, so that $\epsilon = -\Psi = \Delta\omega^2 - k_{ex}^2 > 0$ but is small. Then

$$\begin{aligned}
D_+ &= \frac{\Delta\omega^2}{|\Psi|} = \frac{\Delta\omega^2}{\epsilon} \\
D_- &= -1 + \frac{\Delta\omega^2}{|\Psi|} = \frac{k_{ex}^2}{\epsilon} \\
\lambda_+ &= 0 \\
\lambda_- &= |\Psi|^{1/2} = \epsilon^{1/2}
\end{aligned}$$

Thus

$$\begin{aligned}
D_+cosh(\tau\lambda_+) - D_-cos(\tau\lambda_-) &= \frac{\Delta\omega^2}{\epsilon} - \frac{k_{ex}^2}{\epsilon}cos(\tau\epsilon^{1/2}) \\
&\simeq \frac{1}{\epsilon}((k_{ex}^2 + \epsilon) - k_{ex}^2(1 - \frac{1}{2}\tau^2\epsilon)) \\
&= 1 + \frac{1}{2}k_{ex}^2\tau^2
\end{aligned}$$

And so again

$$R_2 \simeq R_{2max} + \frac{1}{2}k_{ex} - \frac{1}{2\tau}cosh^{-1}(1 + \frac{1}{2}k_{ex}^2\tau^2)$$

So if you can work around the singularity the result is continuous across $\Psi = 0$.

Case: $k_{AB} = k_{BA}$, $\Psi > 0$, derivatives

For the non-linear fitting routine we need the derivatives of R_2 with respect to the parameters R_{2max}, k_{ex} and $\Delta\omega$.

For this case remember that we have

$$\begin{aligned}
D_+ &= 1 + \frac{\Delta\omega^2}{\Psi} = \frac{k_{ex}^2}{\Psi} \\
D_- &= \frac{\Delta\omega^2}{\Psi} \\
\lambda_+ &= \Psi^{1/2} \\
\lambda_- &= 0 \\
\Psi &= k_{ex}^2 - \Delta\omega^2
\end{aligned}$$

Thus

$$R_2 = R_{2max} + \frac{1}{2}k_{ex} - \frac{1}{2\tau}cosh^{-1}(D_+cosh(\tau\lambda_+) - D_-)$$

The trivial derivative is

$$\frac{\partial R_2}{\partial R_{2max}} = 1$$

Note that

$$\frac{d}{dx}cosh^{-1}(x) = \frac{1}{\sqrt{x^2-1}}$$

Let

$$v = D_+cosh(\tau\lambda_+) - D_-$$

Then

$$\begin{aligned}
\frac{\partial R_2}{\partial k_{ex}} &= \frac{1}{2} - \frac{1}{2\tau}\frac{1}{\sqrt{v^2-1}}\frac{\partial v}{\partial k_{ex}} \\
\frac{\partial v}{\partial k_{ex}} &= \frac{\partial D_+}{\partial k_{ex}}cosh(\tau\lambda_+) + D_+\tau sinh(\tau\lambda_+)\frac{\partial \lambda_+}{\partial k_{ex}} - \frac{\partial D_-}{\partial k_{ex}} \\
\frac{\partial D_+}{\partial k_{ex}} &= \frac{\partial D_-}{\partial k_{ex}} = -\frac{2k_{ex}\Delta\omega^2}{\Psi^2} \\
\frac{\partial \lambda_+}{\partial k_{ex}} &= k_{ex}\Psi^{-1/2}
\end{aligned}$$

And

$$\begin{aligned}
\frac{\partial R_2}{\partial \Delta\omega} &= -\frac{1}{2\tau}\frac{1}{\sqrt{v^2-1}}\frac{\partial v}{\partial \Delta\omega} \\
\frac{\partial v}{\partial \Delta\omega} &= \frac{\partial D_+}{\partial \Delta\omega}cosh(\tau\lambda_+) + D_+\tau sinh(\tau\lambda_+)\frac{\partial \lambda_+}{\partial \Delta\omega} - \frac{\partial D_-}{\partial \Delta\omega} \\
\frac{\partial D_+}{\partial \Delta\omega} &= \frac{\partial D_-}{\partial \Delta\omega} = \frac{2k_{ex}^2\Delta\omega}{\Psi^2} \\
\frac{\partial \lambda_+}{\partial \Delta\omega} &= -\Delta\omega\Psi^{-1/2}
\end{aligned}$$

Case: $k_{AB} = k_{BA}$, $\Psi < 0$, derivatives

For the non-linear fitting routine we need the derivatives of R_2 with respect to the parameters R_{2max}, k_{ex} and $\Delta\omega$.

For this case remember that we have

$$
\begin{aligned}
D_+ &= \frac{\Delta\omega^2}{|\Psi|} \\
D_- &= -1 + \frac{\Delta\omega^2}{|\Psi|} = \frac{k_{ex}^2}{|\Psi|} \\
\lambda_+ &= 0 \\
\lambda_- &= |\Psi|^{1/2} \\
|\Psi| &= \Delta\omega^2 - k_{ex}^2
\end{aligned}
$$

Thus

$$R_2 = R_{2max} + \frac{1}{2}k_{ex} - \frac{1}{2\tau}cosh^{-1}(D_+ - D_-cos(\tau\lambda_-))$$

The trivial derivative is

$$\frac{\partial R_2}{\partial R_{2max}} = 1$$

Let

$$v = D_+ - D_-cos(\tau\lambda_-)$$

Then

$$
\begin{aligned}
\frac{\partial R_2}{\partial k_{ex}} &= \frac{1}{2} - \frac{1}{2\tau}\frac{1}{\sqrt{v^2-1}}\frac{\partial v}{\partial k_{ex}} \\
\frac{\partial v}{\partial k_{ex}} &= \frac{\partial D_+}{\partial k_{ex}} - \frac{\partial D_-}{\partial k_{ex}}cos(\tau\lambda_-) + D_-\tau sin(\tau\lambda_-)\frac{\partial \lambda_-}{\partial k_{ex}} \\
\frac{\partial D_+}{\partial k_{ex}} &= \frac{\partial D_-}{\partial k_{ex}} = \frac{2k_{ex}\Delta\omega^2}{\Psi^2} \\
\frac{\partial \lambda_-}{\partial k_{ex}} &= -k_{ex}|\Psi|^{-1/2}
\end{aligned}
$$

And

$$
\begin{aligned}
\frac{\partial R_2}{\partial \Delta\omega} &= -\frac{1}{2\tau}\frac{1}{\sqrt{v^2-1}}\frac{\partial v}{\partial \Delta\omega} \\
\frac{\partial v}{\partial \Delta\omega} &= \frac{\partial D_+}{\partial \Delta\omega} - \frac{\partial D_-}{\partial \Delta\omega} cos(\tau\lambda_-) + D_-\tau sin(\tau\lambda_-)\frac{\partial \lambda_-}{\partial \Delta\omega} \\
\frac{\partial D_+}{\partial \Delta\omega} &= \frac{\partial D_-}{\partial \Delta\omega} = -\frac{2k_{ex}^2\Delta\omega}{\Psi^2} \\
\frac{\partial \lambda_-}{\partial \Delta\omega} &= \Delta\omega|\Psi|^{-1/2}
\end{aligned}
$$

Case: $k_{AB} \neq k_{BA}$, derivatives

For the non-linear fitting routine we need the derivatives of R_2 with respect to the parameters R_{2max}, k_{AB}, k_{BA} and $\Delta\omega$.

The trivial derivative is

$$
\frac{\partial R_2}{\partial R_{2max}} = 1
$$

Let

$$
v = D_+ cosh(\tau\lambda_+) - D_- cos(\tau\lambda_-)
$$

Then

$$
\begin{aligned}
\frac{\partial R_2}{\partial k_{AB}} &= \frac{1}{2} - \frac{1}{2\tau}\frac{1}{\sqrt{v^2-1}}\frac{\partial v}{\partial k_{AB}} \\
\frac{\partial v}{\partial k_{AB}} &= \frac{\partial D_+}{\partial k_{AB}} cosh(\tau\lambda_+) + D_+\tau sinh(\tau\lambda_+)\frac{\partial \lambda_+}{\partial k_{AB}} - \frac{\partial D_-}{\partial k_{AB}} cos(\tau\lambda_-) + D_-\tau sin(\tau\lambda_-)\frac{\partial \lambda_-}{\partial k_{AB}} \\
\frac{\partial D_\pm}{\partial k_{AB}} &= \frac{k_{ex}}{(\Psi^2+\zeta^2)^{1/2}} - \frac{(\Psi+2\Delta\omega^2)(\Psi k_{ex}+\zeta\Delta\omega)}{(\Psi^2+\zeta^2)^{3/2}} \\
\frac{\partial \lambda_\pm}{\partial k_{AB}} &= \frac{1}{2\lambda_\pm}\left(\pm k_{ex} + \frac{\Psi k_{ex}+\zeta\Delta\omega}{(\Psi^2+\zeta^2)^{1/2}}\right)
\end{aligned}
$$

And

$$
\begin{aligned}
\frac{\partial R_2}{\partial k_{BA}} &= \frac{1}{2} - \frac{1}{2\tau}\frac{1}{\sqrt{v^2-1}}\frac{\partial v}{\partial k_{BA}} \\
\frac{\partial v}{\partial k_{BA}} &= \frac{\partial D_+}{\partial k_{BA}} cosh(\tau\lambda_+) + D_+\tau sinh(\tau\lambda_+)\frac{\partial \lambda_+}{\partial k_{BA}} - \frac{\partial D_-}{\partial k_{BA}} cos(\tau\lambda_-) + D_-\tau sin(\tau\lambda_-)\frac{\partial \lambda_-}{\partial k_{BA}} \\
\frac{\partial D_\pm}{\partial k_{BA}} &= \frac{k_{ex}}{(\Psi^2+\zeta^2)^{1/2}} - \frac{(\Psi+2\Delta\omega^2)(\Psi k_{ex}-\zeta\Delta\omega)}{(\Psi^2+\zeta^2)^{3/2}} \\
\frac{\partial \lambda_\pm}{\partial k_{BA}} &= \frac{1}{2\lambda_\pm}\left(\pm k_{ex} + \frac{\Psi k_{ex}-\zeta\Delta\omega}{(\Psi^2+\zeta^2)^{1/2}}\right)
\end{aligned}
$$

And

$$
\begin{aligned}
\frac{\partial R_2}{\partial \Delta\omega} &= -\frac{1}{2\tau}\frac{1}{\sqrt{v^2-1}}\frac{\partial v}{\partial \Delta\omega} \\
\frac{\partial v}{\partial \Delta\omega} &= \frac{\partial D_+}{\partial \Delta\omega} cosh(\tau\lambda_+) + D_+ \tau sinh(\tau\lambda_+)\frac{\partial \lambda_+}{\partial \Delta\omega} - \frac{\partial D_-}{\partial \Delta\omega} cos(\tau\lambda_-) + D_- \tau sin(\tau\lambda_-)\frac{\partial \lambda_-}{\partial \Delta\omega} \\
\frac{\partial D_\pm}{\partial \Delta\omega} &= \frac{\Delta\omega}{(\Psi^2+\zeta^2)^{1/2}} \; - \; \frac{(\Psi + 2\Delta\omega^2)(-\Psi\Delta\omega + \zeta(k_{AB}-k_{BA}))}{(\Psi^2+\zeta^2)^{3/2}} \\
\frac{\partial \lambda_\pm}{\partial \Delta\omega} &= \frac{1}{2\lambda_\pm}\left(\mp\Delta\omega + \frac{-\Psi\Delta\omega + \zeta(k_{AB}-k_{BA})}{(\Psi^2+\zeta^2)^{1/2}}\right)
\end{aligned}
$$