Supplemental Material

Mathematica Notebooks

General expressions for $R_{1\rho}$ relaxation for *N*-site chemical exchange and the special case of linear chains

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The following document contains printouts of the Mathematica notebooks entitled:

twosite_allcalculations.nb
threesite_allcalculations.nb
foursite_allcalculations.nb

and is intended for readers who are unable to open the actual mathematic notebook files.

This defines some L, I, and R matrices (or a combination of L+R), deltaR, some rate constants - note that k32ex=k23ft+k32ft (and similar). k13ftl and k13ft (and similar) only differ in that k13ftl does not contain a dummy k32ex_ variable. Herein, theta, cos2(theta), sinsq(theta) are also defined in this block.

```
In[780]:= Off[General::luc]
I3 = IdentityMatrix[3];
BigI = ArrayFlatten[{{I3, 0 I3, 0 I3}, {0 I3, I3, 0 I3}, {0 I3, 0 I3, I3}}];
MatrixForm[BigI]
LA = {{0, -WA, 0}, {WA, 0, -w1}, {0, w1, 0}};
LC = {{0, -WC, 0}, {WC, 0, -w1}, {0, w1, 0}};
LB = {{0, -WB, 0}, {WB, 0, -w1}, {0, w1, 0}};
MatrixForm[LA];
MatrixForm[LC];
MatrixForm[LB];
BigLtr[WA_, WB_, WC_, w1_] =
  ArrayFlatten[{{LA, 0 I3, 0 I3}, {0 I3, LB, 0 I3}, {0 I3, 0 I3, LC}}];
MatrixForm[BigLtr[WA, WB, WC, w1]]
RAr = {{0, 0, 0}, {0, 0, 0}, {0, 0, R2 - R1}};
RBr = {{0, 0, 0}, {0, 0, 0}, {0, 0, R2 - R1}};
RCr = {{0, 0, 0}, {0, 0, 0}, {0, 0, R2 - R1}};
BigDRr[R1_, R2_] =
 ArrayFlatten[{{RAr, 0 I3, 0 I3}, {0 I3, RBr, 0 I3}, {0 I3, 0 I3, RCr}}]
MatrixForm[BigDRr[R1, R2]]
LAr = {{-R2, -WA, 0}, {WA, -R2, -w1}, {0, w1, -R1}};
LBr = {{-R2, -WB, 0}, {WB, -R2, -w1}, {0, w1, -R1}};
LCr = {{-R2, -WC, 0}, {WC, -R2, -w1}, {0, w1, -R1}};
BigLtrr[R1_, R2_, WA_, WB_, WC_, w1_] =
 ArrayFlatten[{{LAr, 0 I3, 0 I3}, {0 I3, LBr, 0 I3}, {0 I3, 0 I3, LCr}}]
MatrixForm[BigLtrr[R1, R2, WA, WB, WC, w1]]
theta[DELTAO_, WB_, WC_, w1_, Pa_, Pb_, Pc_] :=
  ArcSin[Sqrt[(w1^2) / (w1^2 + (Pa * (DELTAO - Pb * WB - Pc * WC) + Pb *
          (WB + (DELTAO - Pb * WB - Pc * WC)) + Pc * (WC + DELTAO - Pb * WB - Pc * WC)) ^2)]];
cossq[DELTAO_, WB_, WC_, w1_, Pa_, Pb_, Pc_] :=
  Cos[theta[DELTAO, WB, WC, w1, Pa, Pb, Pc]]^2;
sinsq[DELTAO_, WB_, WC_, w1_, Pa_, Pb_, Pc_] :=
  Sin[theta[DELTAO, WB, WC, w1, Pa, Pb, Pc]]^2;
k23ft[k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_] = k32ex / (1 + Pb / Pc);
k13ft[k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_] = k31ex / (1 + Pa / Pc);
k12ft[k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_] = k21ex / (1 + Pa / Pb);
k32ft[k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_] = k32ex - k32ex / (1 + Pb / Pc);
k31ft[k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_] = k31ex - k31ex / (1 + Pa / Pc);
k21ft[k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_] = k21ex - k21ex / (1 + Pa / Pb);
k13ftl[k21ex_, k31ex_, Pa_, Pb_, Pc_] = k31ex / (1 + Pa / Pc);
k12ftl[k21ex_, k31ex_, Pa_, Pb_, Pc_] = k21ex / (1 + Pa / Pb);
k31ftl[k21ex_, k31ex_, Pa_, Pb_, Pc_] = k31ex - k31ex / (1 + Pa / Pc);
k21ftl[k21ex_, k31ex_, Pa_, Pb_, Pc_] = k21ex - k21ex / (1 + Pa / Pb);
```

Out[783]//MatrixForm=

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

Out[791]//MatrixForm=

$$\begin{pmatrix} 0 & -WA & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ WA & 0 & -w1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & w1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -WB & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & WB & 0 & -w1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & w1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -WC & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & WC & 0 & -w1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & w1 & 0 \end{pmatrix}$$

Out[795]=
```
{{0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, -R1 + R2, 0, 0, 0, 0, 0, 0},
 {0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, -R1 + R2, 0, 0, 0},
 {0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, -R1 + R2}}
```

Out[796]//MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -R1+R2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -R1+R2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -R1+R2 \end{pmatrix}$$

Out[800]=
```
{{-R2, -WA, 0, 0, 0, 0, 0, 0, 0},
 {WA, -R2, -w1, 0, 0, 0, 0, 0, 0}, {0, w1, -R1, 0, 0, 0, 0, 0, 0},
 {0, 0, 0, -R2, -WB, 0, 0, 0, 0}, {0, 0, 0, WB, -R2, -w1, 0, 0, 0},
 {0, 0, 0, 0, w1, -R1, 0, 0, 0}, {0, 0, 0, 0, 0, 0, -R2, -WC, 0},
 {0, 0, 0, 0, 0, 0, WC, -R2, -w1}, {0, 0, 0, 0, 0, 0, 0, w1, -R1}}
```

Out[801]//MatrixForm=

$$\begin{pmatrix} -R2 & -WA & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ WA & -R2 & -w1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & w1 & -R1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -R2 & -WB & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & WB & -R2 & -w1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & w1 & -R1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -R2 & -WC & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & WC & -R2 & -w1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & w1 & -R1 \end{pmatrix}$$

K matrices for 3-site linear and triangular schemes are produces. Matrices and expressions for the Woodbury approximation are defined.
First order approximations (Eq. 11) and expressions to obtain numerical (least negative eigenvalue) results for linear and triangular schemes are defined.

In[815]:=

```
Ktriangular[k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_] = ArrayFlatten[
```

```
    {{(-k12ft[k21ex, k31ex, k32ex, Pa, Pb, Pc] - k13ft[k21ex, k31ex, k32ex, Pa, Pb, Pc])
       I3, k21ft[k21ex, k31ex, k32ex, Pa, Pb, Pc] I3,
      k31ft[k21ex, k31ex, k32ex, Pa, Pb, Pc] I3},
     {k12ft[k21ex, k31ex, k32ex, Pa, Pb, Pc] I3,
      (-k21ft[k21ex, k31ex, k32ex, Pa, Pb, Pc] - k23ft[k21ex, k31ex, k32ex, Pa, Pb, Pc])
       I3, k32ft[k21ex, k31ex, k32ex, Pa, Pb, Pc] I3},
     {k13ft[k21ex, k31ex, k32ex, Pa, Pb, Pc] I3, k23ft[k21ex, k31ex, k32ex, Pa, Pb, Pc]
       I3, (-k31ft[k21ex, k31ex, k32ex, Pa, Pb, Pc] -
         k32ft[k21ex, k31ex, k32ex, Pa, Pb, Pc]) I3}}];
Klinear[k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_] = ArrayFlatten[
    {{(-k12ft[k21ex, k31ex, k32ex, Pa, Pb, Pc] - k13ft[k21ex, k31ex, k32ex, Pa, Pb, Pc])
       I3, k21ft[k21ex, k31ex, k32ex, Pa, Pb, Pc] I3,
      k31ft[k21ex, k31ex, k32ex, Pa, Pb, Pc] I3},
     {k12ft[k21ex, k31ex, k32ex, Pa, Pb, Pc] I3,
      -k21ft[k21ex, k31ex, k32ex, Pa, Pb, Pc] I3, 0 I3},
     {k13ft[k21ex, k31ex, k32ex, Pa, Pb, Pc] I3, 0 I3,
      -k31ft[k21ex, k31ex, k32ex, Pa, Pb, Pc] I3}}];
Umat = ArrayFlatten[{{0 I3}, {I3}, {-I3}}];
MatrixForm[Umat]
Vmat[k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_] =
  ArrayFlatten[{{0 I3, -k23ft[k21ex, k31ex, k32ex, Pa, Pb, Pc] I3,
     k32ft[k21ex, k31ex, k32ex, Pa, Pb, Pc] I3}}];
MatrixForm[Vmat[k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_]]
MatrixForm[Klinear[k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_]]
MatrixForm[Ktriangular[k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_]]
InvLK[DELTAO_, WB_, WC_, w1_, k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_] :=
  Inverse[BigLtr[DELTAO - Pb * WB - Pc * WC, WB + (DELTAO - Pb * WB - Pc * WC),
     WC + (DELTAO - Pb * WB - Pc * WC), w1] + Klinear[k21ex, k31ex, k32ex, Pa, Pb, Pc]];
ZWoodbury[DELTAO_, WB_, WC_, w1_, k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_] :=
 Tr[InvLK[DELTAO, WB, WC, w1, k21ex, k31ex, k32ex, Pa, Pb, Pc].Umat.
   Inverse[I3 + Vmat[k21ex, k31ex, k32ex, Pa, Pb, Pc].InvLK[DELTAO, WB, WC, w1, k21ex,
       k31ex, k32ex, Pa, Pb, Pc].Umat].Vmat[k21ex, k31ex, k32ex, Pa, Pb, Pc].
   InvLK[DELTAO, WB, WC, w1, k21ex, k31ex, k32ex, Pa, Pb, Pc]]

threelinearfirstorder[DELTAO_, WB_,
   WC_, w1_, k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_] :=
  - (1 / Tr[Inverse[BigLtr[DELTAO - Pb * WB - Pc * WC, WB + (DELTAO - Pb * WB - Pc * WC),
          WC + (DELTAO - Pb * WB - Pc * WC), w1] + Klinear[k21ex, k31ex,
          k32ex, Pa, Pb, Pc]]]) / sinsq[DELTAO, WB, WC, w1, Pa, Pb, Pc];
threetriangularfirstorder[DELTAO_, WB_, WC_, w1_, k21ex_, k31ex_,
   k32ex_, Pa_, Pb_, Pc_] :=
  - (1 / Tr[Inverse[BigLtr[DELTAO - Pb * WB - Pc * WC, WB + (DELTAO - Pb * WB - Pc * WC),
          WC + (DELTAO - Pb * WB - Pc * WC), w1] + Ktriangular[k21ex, k31ex,
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            k32ex, Pa, Pb, Pc]]]) / sinsq[DELTAO, WB, WC, w1, Pa, Pb, Pc];
threetriangularexact[DELTAO_, WB_, WC_, w1_, k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_] :=
  -N[Re[Eigenvalues[
        Ktriangular[k21ex, k31ex, k32ex, Pa, Pb, Pc] + BigLtr[DELTAO - Pb * WB - Pc * WC,
          WB + (DELTAO - Pb * WB - Pc * WC), WC + (DELTAO - Pb * WB - Pc * WC), w1]]]][[
      9]] / sinsq[DELTAO, WB, WC, w1, Pa, Pb, Pc];
threelinearexact[DELTAO_, WB_, WC_, w1_, k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_] :=
  -N[Re[Eigenvalues[
        Klinear[k21ex, k31ex, k32ex, Pa, Pb, Pc] + BigLtr[DELTAO - Pb * WB - Pc * WC,
          WB + (DELTAO - Pb * WB - Pc * WC), WC + (DELTAO - Pb * WB - Pc * WC), w1]]]][[
      9]] / sinsq[DELTAO, WB, WC, w1, Pa, Pb, Pc];
```

Out[818]//MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Out[820]//MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 & -\frac{k32ex\_}{1+\frac{Pb\_}{Pc\_}} & 0 & 0 & k32ex\_ - \frac{k32ex\_}{1+\frac{Pb\_}{Pc\_}} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{k32ex\_}{1+\frac{Pb\_}{Pc\_}} & 0 & 0 & k32ex\_ - \frac{k32ex\_}{1+\frac{Pb\_}{Pc\_}} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{k32ex\_}{1+\frac{Pb\_}{Pc\_}} & 0 & 0 & k32ex\_ - \frac{k32ex\_}{1+\frac{Pb\_}{Pc\_}} \end{pmatrix}$$

Out[821]//MatrixForm=

$$\begin{pmatrix} -\frac{k21ex\_}{1+\frac{Pa\_}{Pb\_}} - \frac{k31ex\_}{1+\frac{Pa\_}{Pc\_}} & 0 & 0 & k21ex\_ - \frac{k21ex\_}{1+\frac{Pa\_}{Pb\_}} & 0 & 0 \\ 0 & -\frac{k21ex\_}{1+\frac{Pa\_}{Pb\_}} - \frac{k31ex\_}{1+\frac{Pa\_}{Pc\_}} & 0 & 0 & k21ex\_ - \frac{k21ex\_}{1+\frac{Pa\_}{Pb\_}} & 0 \\ 0 & 0 & -\frac{k21ex\_}{1+\frac{Pa\_}{Pb\_}} - \frac{k31ex\_}{1+\frac{Pa\_}{Pc\_}} & 0 & 0 & k21ex\_ - \frac{k2}{1+} \\ \frac{k21ex\_}{1+\frac{Pa\_}{Pb\_}} & 0 & 0 & -k21ex\_ + \frac{k21ex\_}{1+\frac{Pa\_}{Pb\_}} & 0 & 0 \\ 0 & \frac{k21ex\_}{1+\frac{Pa\_}{Pb\_}} & 0 & 0 & -k21ex\_ + \frac{k21ex\_}{1+\frac{Pa\_}{Pb\_}} & 0 \\ 0 & 0 & \frac{k21ex\_}{1+\frac{Pa\_}{Pb\_}} & 0 & 0 & -k21ex\_ + \frac{k2}{1} \\ \frac{k31ex\_}{1+\frac{Pa\_}{Pc\_}} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{k31ex\_}{1+\frac{Pa\_}{Pc\_}} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{k31ex\_}{1+\frac{Pa\_}{Pc\_}} & 0 & 0 & 0 \end{pmatrix}$$

Out[822]//MatrixForm=

$$\begin{pmatrix}
-\frac{k21ex_}{1+\frac{Pa_}{Pb_}}-\frac{k31ex_}{1+\frac{Pa_}{Pc_}} & 0 & 0 & k21ex_-\frac{k21ex_}{1+\frac{Pa_}{Pb_}} & 0 \\
0 & -\frac{k21ex_}{1+\frac{Pa_}{Pb_}}-\frac{k31ex_}{1+\frac{Pa_}{Pc_}} & 0 & 0 & k21ex_-\frac{k21ex_}{1+\frac{Pa_}{Pb_}} \\
0 & 0 & -\frac{k21ex_}{1+\frac{Pa_}{Pb_}}-\frac{k31ex_}{1+\frac{Pa_}{Pc_}} & 0 & 0 \\
\frac{k21ex_}{1+\frac{Pa_}{Pb_}} & 0 & 0 & -k21ex_+\frac{k21ex_}{1+\frac{Pa_}{Pb_}}-\frac{k32ex_}{1+\frac{Pb_}{Pc_}} & 0 \\
0 & \frac{k21ex_}{1+\frac{Pa_}{Pb_}} & 0 & 0 & -k21ex_+\frac{k21ex_}{1+\frac{Pa_}{Pb_}}-\frac{k32e}{1+\frac{Pb}{Pc}} \\
0 & 0 & \frac{k21ex_}{1+\frac{Pa_}{Pb_}} & 0 & 0 \\
\frac{k31ex_}{1+\frac{Pa_}{Pc_}} & 0 & 0 & \frac{k32ex_}{1+\frac{Pb_}{Pc_}} & 0 \\
0 & \frac{k31ex_}{1+\frac{Pa_}{Pc_}} & 0 & 0 & \frac{k32ex_}{1+\frac{Pb_}{Pc_}} \\
0 & 0 & \frac{k31ex_}{1+\frac{Pa_}{Pc_}} & 0 & 0
\end{pmatrix}$$

The following calculates a second order approximation of Rex for a 3-state linear kinetic scheme. (Eqs. 24, 35-40). L defined slightly differently from above, for input convenience.

In[829]:=
```
LAy[DELTAO_, WB_, WC_, w1_, Pa_, Pb_, Pc_] =
  {{0, -(DELTAO - Pb * WB - Pc * WC), 0}, {(DELTAO - Pb * WB - Pc * WC), 0, -w1}, {0, w1, 0}};
LBy[DELTAO_, WB_, WC_, w1_, Pa_, Pb_, Pc_] = {{0, -(WB + DELTAO - Pb * WB - Pc * WC), 0},
   {WB + DELTAO - Pb * WB - Pc * WC, 0, -w1}, {0, w1, 0}};
LCy[DELTAO_, WB_, WC_, w1_, Pa_, Pb_, Pc_] = {{0, -(WC + DELTAO - Pb * WB - Pc * WC), 0},
   {WC + DELTAO - Pb * WB - Pc * WC, 0, -w1}, {0, w1, 0}};
MatrixForm[LAy[DELTAO_, WB_, WC_, w1_, Pa_, Pb_, Pc_]]
MatrixForm[LBy[DELTAO_, WB_, WC_, w1_, Pa_, Pb_, Pc_]]
MatrixForm[LCy[DELTAO_, WB_, WC_, w1_, Pa_, Pb_, Pc_]]
LAz[DELTAO_, WB_, WC_, w1_, Pa_, Pb_, Pc_, k21ex_, k31ex_] =
  LAy[DELTAO, WB, WC, w1, Pa, Pb, Pc] -
   (k12ftl[k21ex, k31ex, Pa, Pb, Pc] + k13ftl[k21ex, k31ex, Pa, Pb, Pc]) * I3;
LBz[DELTAO_, WB_, WC_, w1_, Pa_, Pb_, Pc_, k21ex_, k31ex_] =
  LBy[DELTAO, WB, WC, w1, Pa, Pb, Pc] - k21ftl[k21ex, k31ex, Pa, Pb, Pc] * I3;
LCz[DELTAO_, WB_, WC_, w1_, Pa_, Pb_, Pc_, k21ex_, k31ex_] =
  LCy[DELTAO, WB, WC, w1, Pa, Pb, Pc] - k31ftl[k21ex, k31ex, Pa, Pb, Pc] * I3;
Zmat[DELTAO_, WB_, WC_, w1_, Pa_, Pb_, Pc_, k21ex_, k31ex_] :=
  LBz[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex].LAz[DELTAO, WB, WC, w1, Pa,
      Pb, Pc, k21ex, k31ex].LCz[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex] -
   k13ftl[k21ex, k31ex, Pa, Pb, Pc] * k31ftl[k21ex, k31ex, Pa, Pb, Pc] *
    LBz[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex] -
   k12ftl[k21ex, k31ex, Pa, Pb, Pc] * k21ftl[k21ex, k31ex, Pa, Pb, Pc] *
    LCz[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex];
Xmat[DELTAO_, WB_, WC_, w1_, Pa_, Pb_, Pc_, k21ex_, k31ex_] :=
  LBz[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex].
    LAz[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex] +
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    LAz[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex].LCz[DELTAO, WB, WC, w1, Pa,
      Pb, Pc, k21ex, k31ex] + LBz[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex].
     LCz[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex] -
    ((k12ftl[k21ex, k31ex, Pa, Pb, Pc] * k21ftl[k21ex, k31ex, Pa, Pb, Pc] +
        k13ftl[k21ex, k31ex, Pa, Pb, Pc] * k31ftl[k21ex, k31ex, Pa, Pb, Pc]) * I3);
Ymat[DELTAO_, WB_, WC_, w1_, Pa_, Pb_, Pc_, k21ex_, k31ex_] :=
  LBz[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex] + LAz[DELTAO, WB, WC, w1, Pa,
    Pb, Pc, k21ex, k31ex] + LCz[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex];
threelinearsecondorder[DELTAO_, WB_, WC_, w1_, k21ex_,
   k31ex_, k32ex_, Pa_, Pb_, Pc_] :=
  - (1 / (Tr[Inverse[Zmat[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex]].Xmat[DELTAO,
          WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex]] -
        Tr[Inverse[Zmat[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex]].
           Ymat[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex] +
          Minors[Inverse[Zmat[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex]].
            Xmat[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex]]] /
         Tr[Inverse[Zmat[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex]].
          Xmat[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex]])) /
    sinsq[DELTAO, WB, WC, w1, Pa, Pb, Pc];
```

Out[832]//MatrixForm=

$$\begin{pmatrix} 0 & -DELTAO\_ + Pb\_ WB\_ + Pc\_ WC\_ & 0 \\ DELTAO\_ - Pb\_ WB\_ - Pc\_ WC\_ & 0 & -w1\_ \\ 0 & w1\_ & 0 \end{pmatrix}$$

Out[833]//MatrixForm=

$$\begin{pmatrix} 0 & -DELTAO\_ - WB\_ + Pb\_ WB\_ + Pc\_ WC\_ & 0 \\ DELTAO\_ + WB\_ - Pb\_ WB\_ - Pc\_ WC\_ & 0 & -w1\_ \\ 0 & w1\_ & 0 \end{pmatrix}$$

Out[834]//MatrixForm=

$$\begin{pmatrix} 0 & -DELTAO\_ + Pb\_ WB\_ - WC\_ + Pc\_ WC\_ & 0 \\ DELTAO\_ - Pb\_ WB\_ + WC\_ - Pc\_ WC\_ & 0 & -w1\_ \\ 0 & w1\_ & 0 \end{pmatrix}$$

These are modified equations for a certain R1rho second order approximation (see below, R1rhothreelinearsecondorderReffLRK), replacing L' with L'+R.

```
In[854]:= LAyr[R1_, R2_, DELTAO_, WB_, WC_, w1_, Pa_, Pb_, Pc_] =
   {{-R2, -(DELTAO - Pb * WB - Pc * WC), 0},
    {(DELTAO - Pb * WB - Pc * WC), -R2, -w1}, {0, w1, -R1}};
  LByr[R1_, R2_, DELTAO_, WB_, WC_, w1_, Pa_, Pb_, Pc_] =
   {{-R2, -(WB + DELTAO - Pb * WB - Pc * WC), 0},
    {WB + DELTAO - Pb * WB - Pc * WC, -R2, -w1}, {0, w1, -R1}};
  LCyr[R1_, R2_, DELTAO_, WB_, WC_, w1_, Pa_, Pb_, Pc_] =
   {{-R2, -(WC + DELTAO - Pb * WB - Pc * WC), 0},
    {WC + DELTAO - Pb * WB - Pc * WC, -R2, -w1}, {0, w1, -R1}};
  MatrixForm[LAyr[R1, R2, DELTAO_, WB_, WC_, w1_, Pa_, Pb_, Pc_]]
```

```
MatrixForm[LByr[R1, R2, DELTAO_, WB_, WC_, w1_, Pa_, Pb_, Pc_]]
MatrixForm[LCyr[R1, R2, DELTAO_, WB_, WC_, w1_, Pa_, Pb_, Pc_]]
LAzr[R1_, R2_, DELTAO_, WB_, WC_, w1_, Pa_, Pb_, Pc_, k21ex_, k31ex_] =
  LAyr[R1, R2, DELTAO, WB, WC, w1, Pa, Pb, Pc] -
   (k12ftl[k21ex, k31ex, Pa, Pb, Pc] + k13ftl[k21ex, k31ex, Pa, Pb, Pc]) * I3;
LBzr[R1_, R2_, DELTAO_, WB_, WC_, w1_, Pa_, Pb_, Pc_, k21ex_, k31ex_] =
  LByr[R1, R2, DELTAO, WB, WC, w1, Pa, Pb, Pc] - k21ftl[k21ex, k31ex, Pa, Pb, Pc] * I3;
LCzr[R1_, R2_, DELTAO_, WB_, WC_, w1_, Pa_, Pb_, Pc_, k21ex_, k31ex_] =
  LCyr[R1, R2, DELTAO, WB, WC, w1, Pa, Pb, Pc] - k31ftl[k21ex, k31ex, Pa, Pb, Pc] * I3;

Zmatr[R1_, R2_, DELTAO_, WB_, WC_, w1_, Pa_, Pb_, Pc_, k21ex_, k31ex_] :=
  LBzr[R1, R2, DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex].
    LAzr[R1, R2, DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex].
    LCzr[R1, R2, DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex] -
   k13ftl[k21ex, k31ex, Pa, Pb, Pc] * k31ftl[k21ex, k31ex, Pa, Pb, Pc] *
    LBzr[R1, R2, DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex] -
   k12ftl[k21ex, k31ex, Pa, Pb, Pc] * k21ftl[k21ex, k31ex, Pa, Pb, Pc] *
    LCzr[R1, R2, DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex];
Xmatr[R1_, R2_, DELTAO_, WB_, WC_, w1_, Pa_, Pb_, Pc_, k21ex_, k31ex_] :=
  LBzr[R1, R2, DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex].
    LAzr[R1, R2, DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex] +
   LAzr[R1, R2, DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex].
    LCzr[R1, R2, DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex] +
   LBzr[R1, R2, DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex].
    LCzr[R1, R2, DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex] -
   ((k12ftl[k21ex, k31ex, Pa, Pb, Pc] * k21ftl[k21ex, k31ex, Pa, Pb, Pc] +
       k13ftl[k21ex, k31ex, Pa, Pb, Pc] * k31ftl[k21ex, k31ex, Pa, Pb, Pc]) * I3);
Ymatr[R1_, R2_, DELTAO_, WB_, WC_, w1_, Pa_, Pb_, Pc_, k21ex_, k31ex_] :=
  LBzr[R1, R2, DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex] +
   LAzr[R1, R2, DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex] +
   LCzr[R1, R2, DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex];
```

Out[857]//MatrixForm=

```
( -R2                          -DELTAO_ + Pb_ WB_ + Pc_ WC_    0    )
( DELTAO_ - Pb_ WB_ - Pc_ WC_  -R2                             -w1_ )
( 0                            w1_                             -R1  )
```

Out[858]//MatrixForm=

```
( -R2                                -DELTAO_ - WB_ + Pb_ WB_ + Pc_ WC_    0    )
( DELTAO_ + WB_ - Pb_ WB_ - Pc_ WC_  -R2                                   -w1_ )
( 0                                  w1_                                   -R1  )
```

Out[859]//MatrixForm=

```
( -R2                                -DELTAO_ + Pb_ WB_ - WC_ + Pc_ WC_    0    )
( DELTAO_ - Pb_ WB_ + WC_ - Pc_ WC_  -R2                                   -w1_ )
( 0                                  w1_                                   -R1  )
```

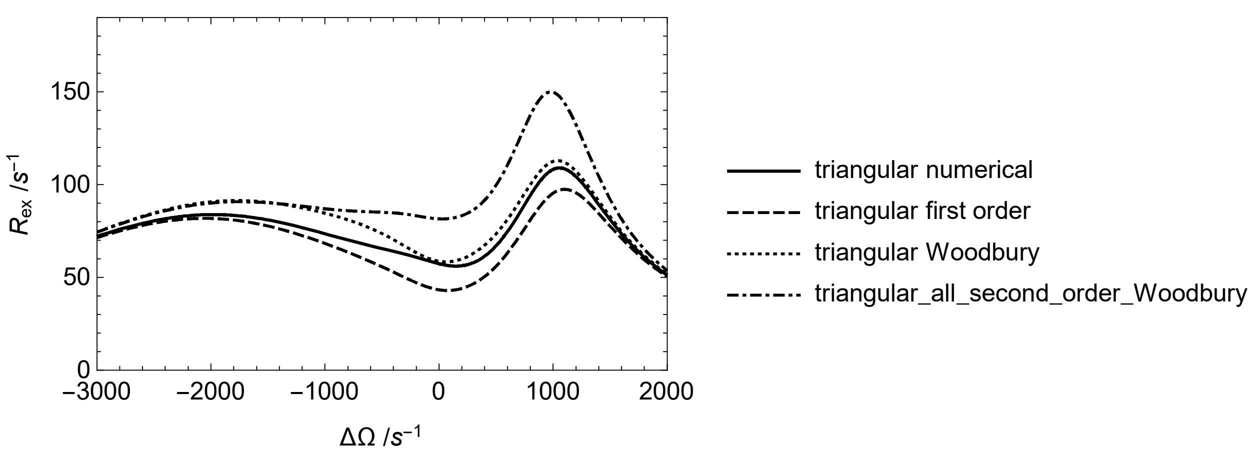
The first (R1rhothreelinearexactr) of the following four equations gives the numerical solution by calculating the least negative of the 9 eigenvalues of the 9 x 9 L+R+K matrix.
R1rhothreelinearsecondorderReffLRK calculates the second order approximation similar to Rex from Eqs. 40 and 29, but replacing L' with L'+R.
R1rhothreelinearsecondorderReffCosSin is Eq. 14; R1rhothreelinearsecondorderReffTrunc is Eq. 10.

```
In[866]:= R1rhothreelinearexactr[R1_, R2_, DELTAO_,
   WB_, WC_, w1_, k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_] :=
  -N[Re[Eigenvalues[Klinear[k21ex, k31ex, k32ex, Pa, Pb, Pc] + BigLtrr[R1,
        R2, DELTAO - Pb * WB - Pc * WC, WB + (DELTAO - Pb * WB - Pc * WC),
        WC + (DELTAO - Pb * WB - Pc * WC), w1]]]]][[9]]
R1rhothreelinearsecondorderReffLRK[R1_, R2_, DELTAO_, WB_, WC_,
   w1_, k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_] :=
  - (1 / (Tr[Inverse[Zmatr[R1, R2, DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex]].
          Xmatr[R1, R2, DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex]] -
        Tr[Inverse[Zmatr[R1, R2, DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex]].
            Ymatr[R1, R2, DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex] +
           Minors[Inverse[Zmatr[R1, R2, DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex]].
             Xmatr[R1, R2, DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex]]] /
         Tr[Inverse[Zmatr[R1, R2, DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex]].
           Xmatr[R1, R2, DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex]]));
R1rhothreelinearsecondorderReffCosSin[R1_, R2_, DELTAO_, WB_, WC_,
   w1_, k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_] :=
  R1 * cossq[DELTAO, WB, WC, w1, Pa, Pb, Pc] + R2 * sinsq[DELTAO, WB, WC, w1, Pa, Pb, Pc] +
   - (1 / (Tr[Inverse[Zmat[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex]].
          Xmat[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex]] -
        Tr[Inverse[Zmat[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex]].
            Ymat[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex] +
           Minors[Inverse[Zmat[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex]].
             Xmat[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex]]] /
         Tr[Inverse[Zmat[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex]].
           Xmat[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex]]))
R1rhothreelinearsecondorderReffTrunc[R1_, R2_, DELTAO_, WB_, WC_,
   w1_, k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_] :=
  R2 - ((Tr[Inverse[BigLtr[DELTAO - Pb * WB - Pc * WC, WB + (DELTAO - Pb * WB - Pc * WC),
             WC + (DELTAO - Pb * WB - Pc * WC), w1] +
           Klinear[k21ex, k31ex, k32ex, Pa, Pb, Pc]].BigDRr[R1, R2]]) /
      Tr[Inverse[BigLtr[DELTAO - Pb * WB - Pc * WC, WB + (DELTAO - Pb * WB - Pc * WC), WC +
            (DELTAO - Pb * WB - Pc * WC), w1] + Klinear[k21ex, k31ex, k32ex, Pa, Pb, Pc]]]) +
   - (1 / (Tr[Inverse[Zmat[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex]].
          Xmat[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex]] -
        Tr[Inverse[Zmat[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex]].
            Ymat[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex] +
           Minors[Inverse[Zmat[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex]].
             Xmat[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex]]] /
         Tr[Inverse[Zmat[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex]].
           Xmat[DELTAO, WB, WC, w1, Pa, Pb, Pc, k21ex, k31ex]]))
```

The following sections plot Figures S5, S3, S2, 5, S5(right panel), 3, S4. Refer to paper for details.
Note that naming of exchange rate constants and states for Fig. 5 is different from the figure caption (but equivalent);
it is more convenient for the calculation to always define k32 to be the non-linear fragment.

In[870]:=
```
WBx = -1000; WCx = 2000; w1x = 500;
k21exx = 50; k31exx = 2000; k32exx = 700;
Pax = 0.85; Pbx = 0.1; Pcx = 0.05;
range1 = -3000; range2 = 2000; rb1 = 0; rb2 = 190
Plot[{threetriangularexact[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx],
  threelinearfirstorder[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx] *
   (1 / (1 + ZWoodbury[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx] *
         threelinearfirstorder[x, WBx, WCx, w1x, k21exx, k31exx, k32exx,
          Pax, Pbx, Pcx] * sinsq[x, WBx, WCx, w1x, Pax, Pbx, Pcx])),
  threelinearsecondorder[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx] *
   (1 / (1 + ZWoodbury[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx] *
         threelinearfirstorder[x, WBx, WCx, w1x, k21exx, k31exx, k32exx,
          Pax, Pbx, Pcx] * sinsq[x, WBx, WCx, w1x, Pax, Pbx, Pcx])),
  threelinearsecondorder[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx] *
   (1 / (1 + ZWoodbury[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx] *
         threelinearsecondorder[x, WBx, WCx, w1x, k21exx, k31exx, k32exx,
          Pax, Pbx, Pcx] * sinsq[x, WBx, WCx, w1x, Pax, Pbx, Pcx]))},
 {x, range1, range2}, GridLines → None, FrameLabel →
  {"ΔΩ /s^-1", "R_ex /s^-1"},
 PlotRange → {{range1, range2}, {rb1, rb2}},
 Axes → None,
 BaseStyle →
  {FontSize → 13},
 Frame → True, PlotTheme → "Monochrome",
 PlotLegends →
  {"triangular numerical", "triangular first order",
   "triangular Woodbury", "triangular_all_second_order_Woodbury"}]
```

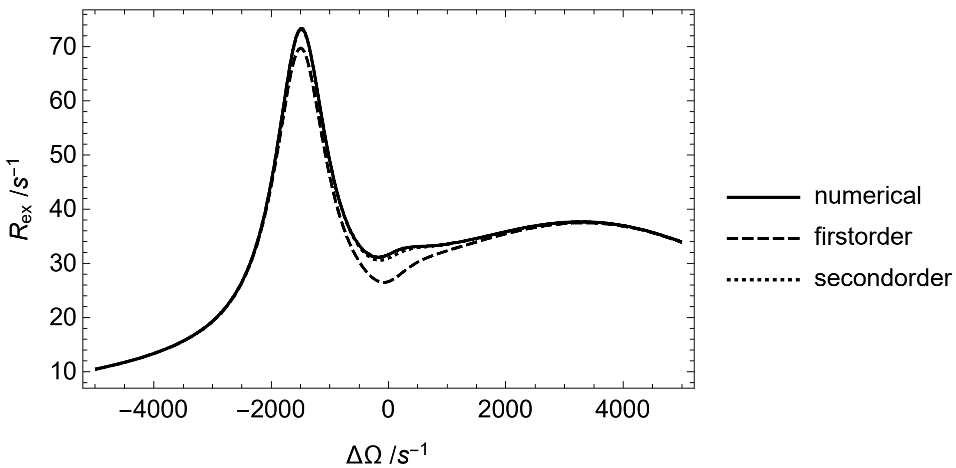
Out[873]= 190

Out[874]=


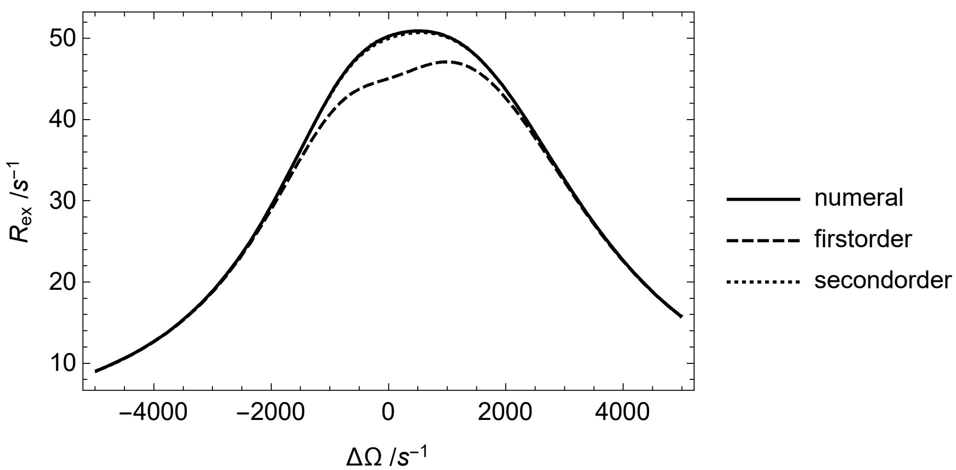
In[875]:=
```
WBx = 1500; WCx = -3500; w1x = 500;
k21exx = 200; k31exx = 5000; k32exx = 0;
Pax = 0.95; Pbx = 0.035; Pcx = 0.015;
range1 = -5000; range2 = 5000; rb1 = 0; rb2 = 80
Plot[{threelinearexact[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx],
  threelinearfirstorder[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx],
  threelinearsecondorder[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx]},
 {x, range1, range2}, GridLines → None, FrameLabel → {"ΔΩ /s^-1", "R_ex /s^-1"},
 PlotRange → Full, Axes → None, BaseStyle → {FontSize → 13}, Frame → True,
 PlotTheme → "Monochrome", PlotLegends → {"numerical", "firstorder", "secondorder"}]
```

Out[878]= 80

Out[879]=



```
In[880]:= WBx = 750; WCx = -1500; w1x = 1250;
k21exx = 1550; k31exx = 2500; k32exx = 0;
Pax = 0.85; Pbx = 0.1; Pcx = 0.05;
range1 = -5000
range2 = 5000
rb1 = 0
rb2 = 80
Plot[{threelinearexact[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx],
  threelinearfirstorder[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx],
  threelinearsecondorder[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx]},
 {x, range1, range2}, GridLines → None, FrameLabel → {"ΔΩ /s^-1", "R_ex /s^-1"},
 PlotRange → Full, Axes → None, BaseStyle → {FontSize → 13}, Frame → True,
 PlotTheme → "Monochrome", PlotLegends → {"numeral", "firstorder", "secondorder"}]
Out[883]= -5000
Out[884]= 5000
Out[885]= 0
Out[886]= 80
```

Out[887]=



```
In[888]:= WBx = 4250; WCx = -4250; w1x = 350;
k21exx = 500; k31exx = 50; k32exx = 20;
Pax = 0.90; Pbx = 0.05; Pcx = 0.05;
range1 = -7000
range2 = 7000
rb1 = 0
rb2 = 1700
Plot[{threetriangularexact[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx],
  threetriangularfirstorder[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx],
  threelinearsecondorder[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx] *
   (1 / (1 + ZWoodbury[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx] *
```

```
threelinearfirstorder[x, WBx, WCx, w1x, k21exx, k31exx, k32exx,
  Pax, Pbx, Pcx] * sinsq[x, WBx, WCx, w1x, Pax, Pbx, Pcx]))},
{x, range1, range2}, GridLines → None, FrameLabel → {"ΔΩ /s^-1", "R_ex /s^-1"},
PlotRange → {{range1, range2}, {rb1, rb2}},
Axes → None,
BaseStyle → {FontSize → 13},
Frame → True,
PlotTheme → "Monochrome",
PlotLegends → {"numerical", "firstorder", "Woodbury"}]
WBx = -4250; WCx = -8500; w1x = 350;
k21exx = 500; k31exx = 20; k32exx = 50;
Pax = 0.05; Pbx = 0.9; Pcx = 0.05;
range1 = -7000
range2 = 7000
rb1 = 0
rb2 = 1700
Plot[{threetriangularexact[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx],
  threetriangularfirstorder[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx],
  threelinearsecondorder[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx] *
   (1 / (1 + ZWoodbury[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx] *
        threelinearfirstorder[x, WBx, WCx, w1x, k21exx, k31exx, k32exx,
         Pax, Pbx, Pcx] * sinsq[x, WBx, WCx, w1x, Pax, Pbx, Pcx]))},
 {x, range1, range2}, GridLines → None, FrameLabel → {"ΔΩ /s^-1", "R_ex /s^-1"},
 PlotRange → {{range1, range2}, {rb1, rb2}},
 Axes → None,
 BaseStyle → {FontSize → 13},
 Frame → True,
 PlotTheme → "Monochrome",
 PlotLegends → {"numerical", "firstorder", "Woodbury"}]
WBx = 8500; WCx = 4250; w1x = 350;
k31exx = 50; k21exx = 20; k32exx = 500;
Pax = 0.05; Pbx = 0.05; Pcx = 0.9;
range1 = -7000
range2 = 7000
rb1 = 0
rb2 = 1700
Plot[{threetriangularexact[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx],
  threetriangularfirstorder[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx],
  threelinearsecondorder[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx] *
   (1 / (1 + ZWoodbury[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx] *
        threelinearfirstorder[x, WBx, WCx, w1x, k21exx, k31exx, k32exx,
         Pax, Pbx, Pcx] * sinsq[x, WBx, WCx, w1x, Pax, Pbx, Pcx]))},
 {x, range1, range2}, GridLines → None, FrameLabel → {"ΔΩ /s^-1", "R_ex /s^-1"},
```

```
PlotRange → {{range1, range2}, {rb1, rb2}},
Axes → None,
BaseStyle → {FontSize → 13},
Frame → True,
PlotTheme → "Monochrome",
PlotLegends → {"numerical", "firstorder", "Woodbury"}]
```

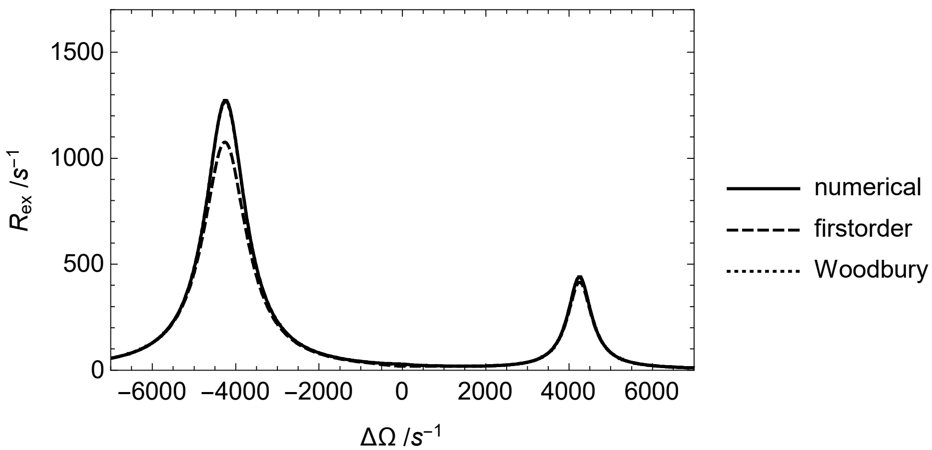
Out[891]= -7000

Out[892]= 7000

Out[893]= 0

Out[894]= 1700

Out[895]=



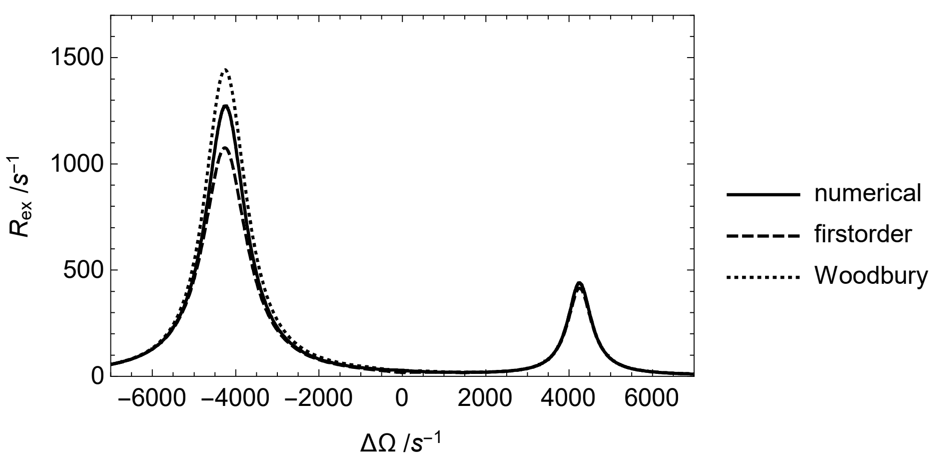
Out[899]= -7000

Out[900]= 7000

Out[901]= 0

Out[902]= 1700

Out[903]=



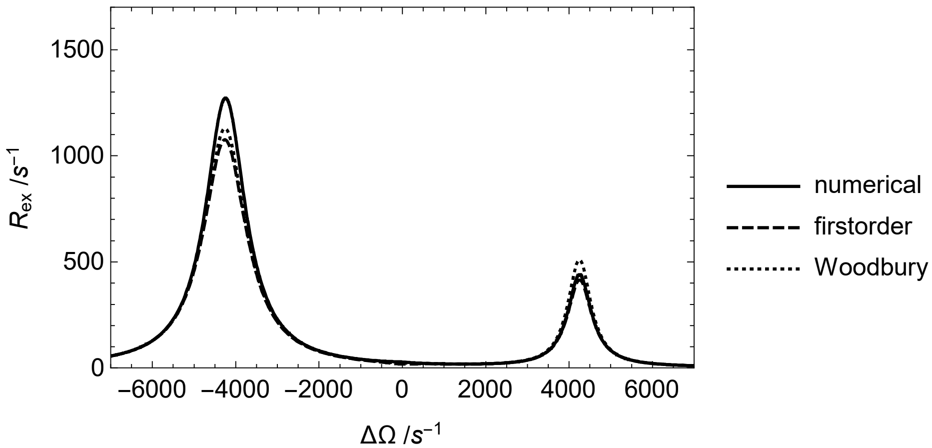
Out[907]= -7000

Out[908]= 7000

Out[909]= 0

Out[910]= 1700

Out[911]=



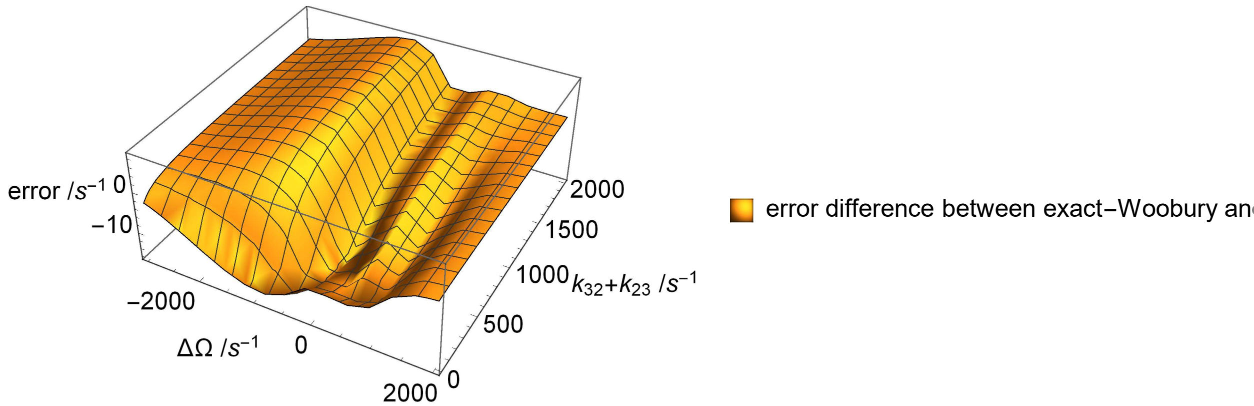
```
WBx = -1000; WCx = 2000; w1x = 500;
k21exx = 50; k31exx = 2000; k32exx = 1000;
Pax = 0.85; Pbx = 0.1; Pcx = 0.05;
range1 = -3000
range2 = 2000
rb1 = 0
rb2 = 300
Plot3D[
 {Abs[(threetriangularexact[x, WBx, WCx, w1x, k21exx, k31exx, y, Pax, Pbx, Pcx] -
      threelinearsecondorder[x, WBx, WCx, w1x, k21exx, k31exx, y, Pax, Pbx, Pcx] *
       (1 / (1 + ZWoodbury[x, WBx, WCx, w1x, k21exx, k31exx, y, Pax, Pbx, Pcx] *
             threelinearfirstorder[x, WBx, WCx, w1x, k21exx, k31exx, y,
              Pax, Pbx, Pcx] * sinsq[x, WBx, WCx, w1x, Pax, Pbx, Pcx])))] -
   Abs[(threetriangularexact[x, WBx, WCx, w1x, k21exx, k31exx, y, Pax, Pbx, Pcx] -
      threelinearfirstorder[x, WBx, WCx, w1x, k21exx, k31exx, y, Pax, Pbx, Pcx] *
       (1 / (1 + ZWoodbury[x, WBx, WCx, w1x, k21exx, k31exx, y, Pax, Pbx, Pcx] *
             threelinearfirstorder[x, WBx, WCx, w1x, k21exx, k31exx, y,
              Pax, Pbx, Pcx] * sinsq[x, WBx, WCx, w1x, Pax, Pbx, Pcx])))]},
 {x, range1, range2}, {y, 10, 2000}, PlotRange →
  All,
 BaseStyle →
  {FontSize → 13},
 AxesLabel →
  {"ΔΩ /s^-1",
   "     k32+k23 /s^-1",
   "error /s^-1"}, PlotLegends →
  {"error difference between exact-Woobury and exact-firstorder
     - smaller means larger first order approx error"}]
```

```
-3000

2000

0

300
```




```
w1x = 50;
k21exx = 50;
k31exx = 100;
k32exx = 0
Pax = 0.52; Pbx = 0.32; Pcx = 0.16;
WBx = 200; WCx = -400;
Plot[{threelinearexact[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx],
   threelinearfirstorder[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx],
   threelinearsecondorder[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx]},
  {x, -1000, 1000}, FrameLabel → {"ΔΩ /s^-1", "Rex /s^-1"}, GridLines → None, Axes → None,
  PlotRange → Full, BaseStyle → {FontSize → 13}, Frame → True, PlotTheme → "Monochrome",
  PlotLegends → {"numerical", "first order", "second order"}]
w1x = 50;
k21exx = 50;
k31exx = 100;
k32exx = 0
Pax = 0.7; Pbx = 0.20; Pcx = 0.10;
WBx = 200; WCx = -400;
Plot[{threelinearexact[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx],
   threelinearfirstorder[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx],
   threelinearsecondorder[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx]},
  {x, -1000, 1000}, FrameLabel → {"ΔΩ /s^-1", "Rex /s^-1"}, GridLines → None, Axes → None,
  PlotRange → Full, BaseStyle → {FontSize → 13}, Frame → True, PlotTheme → "Monochrome",
  PlotLegends → {"numerical", "first order", "second order"}]
w1x = 50;
k21exx = 50;
k31exx = 100;
k32exx = 0
Pax = 0.85; Pbx = 0.10; Pcx = 0.05;
WBx = 200; WCx = -400;
Plot[{threelinearexact[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx],
   threelinearfirstorder[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx],
```

```
    threelinearsecondorder[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx]},
  {x, -1000, 1000}, FrameLabel → {"ΔΩ /s^-1", "R_ex /s^-1"}, GridLines → None, Axes → None,
  PlotRange → Full, BaseStyle → {FontSize → 13}, Frame → True, PlotTheme → "Monochrome",
  PlotLegends → {"numerical", "first order", "second order"}]
w1x = 50;
k21exx = 50;
k31exx = 100;
k32exx = 0
Pax = 0.94; Pbx = 0.04; Pcx = 0.02;
WBx = 200; WCx = -400;
Plot[{threelinearexact[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx],
    threelinearfirstorder[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx],
    threelinearsecondorder[x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx]},
  {x, -1000, 1000}, FrameLabel → {"ΔΩ /s^-1", "R_ex /s^-1"}, GridLines → None, Axes → None,
  PlotRange → Full, BaseStyle → {FontSize → 13}, Frame → True, PlotTheme → "Monochrome",
  PlotLegends → {"numerical", "first order", "second order"}]
```

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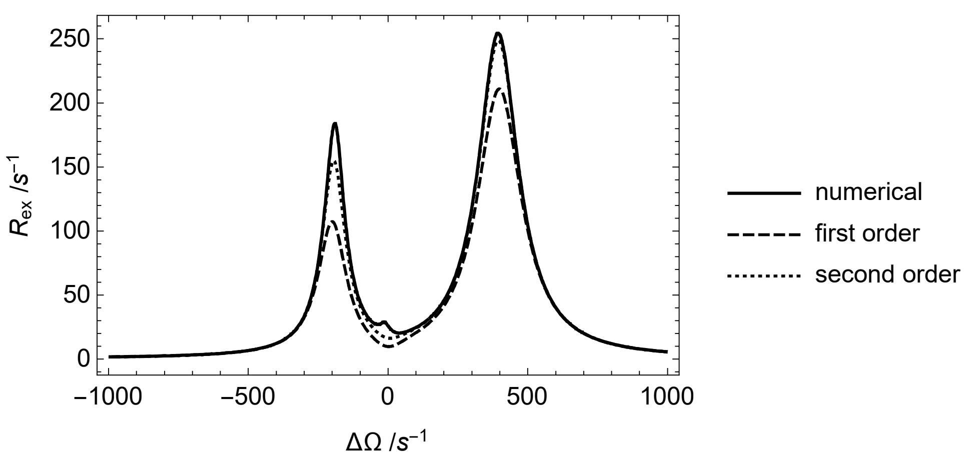

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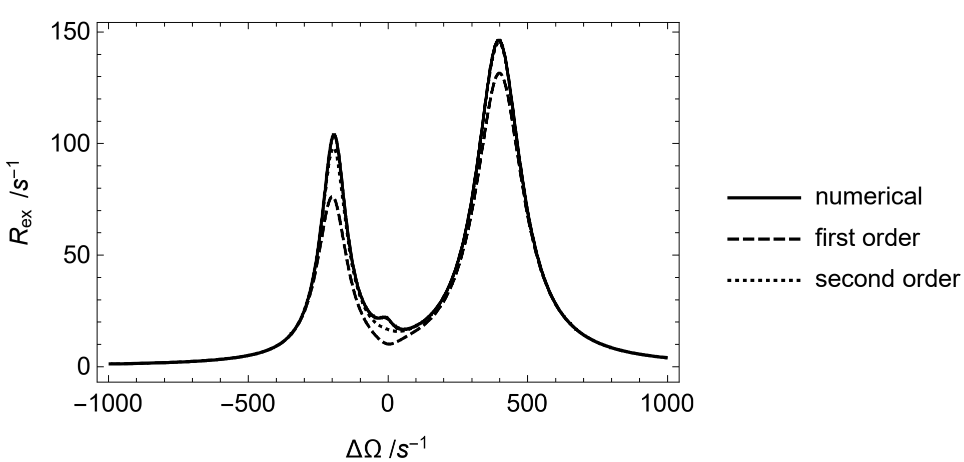

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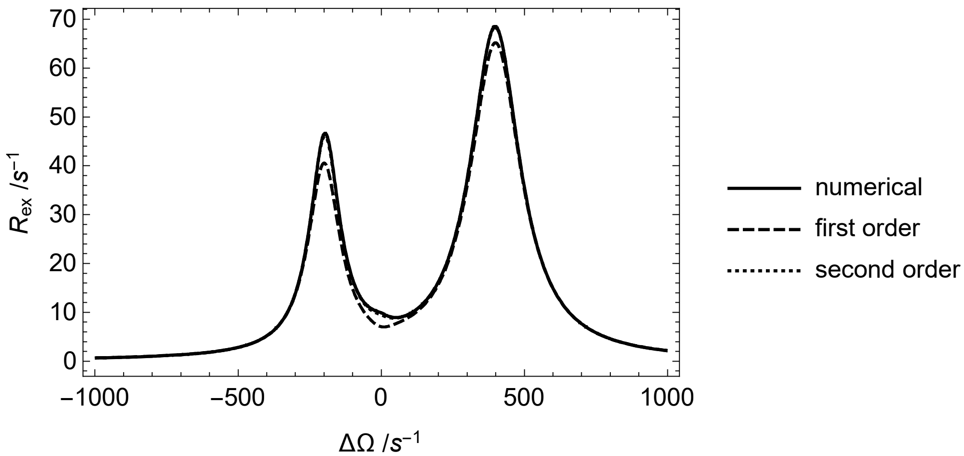

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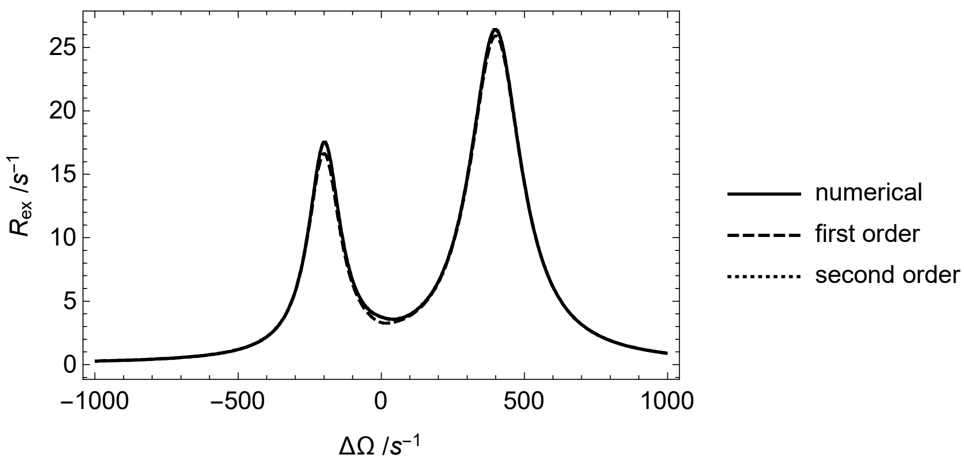
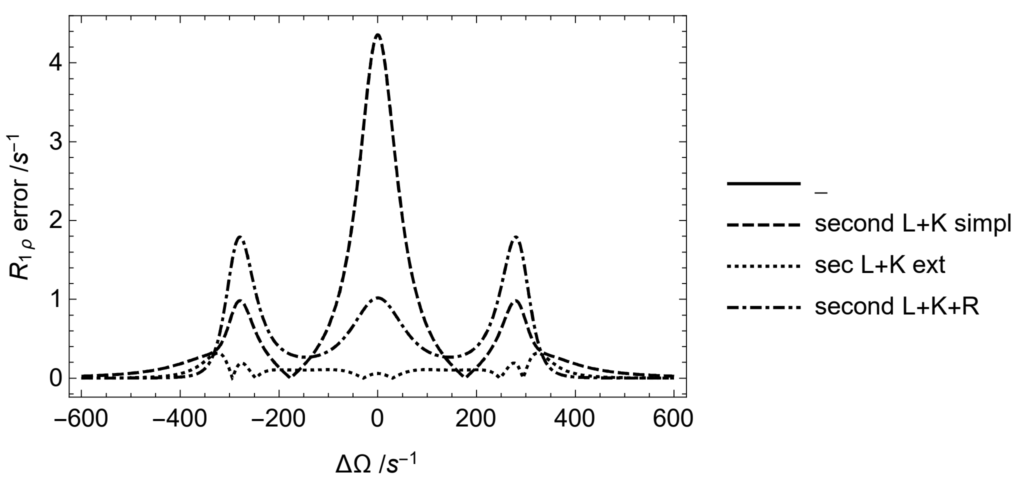


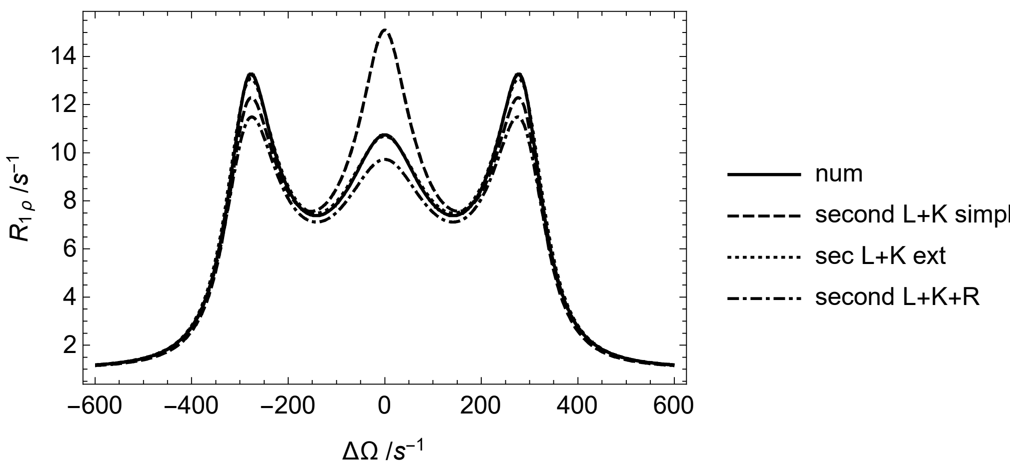

```
R1x = 1; R2x = 6;
w1x = 50;
k21exx = 100;
k31exx = 100;
k32exx = 0;
Pax = 0.3334; Pbx = 0.333; Pcx = 0.333;
WBx = 300; WCx = -300;
a = -600; b = 600;
Plot[
 {uvw, Abs[R1rhothreelinearsecondorderReffCosSin[R1x, R2x, x, WBx, WCx, w1x, k21exx,
     k31exx, k32exx, Pax, Pbx, Pcx] - R1rhothreelinearexactr[R1x,
     R2x, x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx]],
  Abs[R1rhothreelinearsecondorderReffTrunc[R1x, R2x, x, WBx, WCx, w1x,
     k21exx, k31exx, k32exx, Pax, Pbx, Pcx] - R1rhothreelinearexactr[
     R1x, R2x, x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx]],
```

```
   Abs[R1rhothreelinearsecondorderReffLRK[R1x, R2x, x, WBx, WCx, w1x,
       k21exx, k31exx, k32exx, Pax, Pbx, Pcx] - R1rhothreelinearexactr[
       R1x, R2x, x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx]]},
  {x, a, b}, FrameLabel → {"ΔΩ /s^-1", "R1ρ error /s^-1"},
  GridLines → None,
  Axes → None,
  PlotRange → Full,
  BaseStyle → {FontSize → 13},
  Frame → True, PlotTheme → "Monochrome",
  PlotLegends →
   {"_", "second L+K simpl", "sec L+K ext", "second L+K+R", "sec L+K extAGP"}]
R1rhothreelinearexactr[x, 200, -400, 50, 50, 10, 0, 0.7, 0.2, 0.1]
Plot[{R1rhothreelinearexactr[R1x, R2x, x, WBx, WCx, w1x, k21exx,
    k31exx, k32exx, Pax, Pbx, Pcx], R1rhothreelinearsecondorderReffCosSin[
    R1x, R2x, x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx],
   R1rhothreelinearsecondorderReffTrunc[R1x, R2x, x, WBx, WCx, w1x, k21exx,
    k31exx, k32exx, Pax, Pbx, Pcx], R1rhothreelinearsecondorderReffLRK[
    R1x, R2x, x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx]},
  {x, a, b}, FrameLabel → {"ΔΩ /s^-1", "R1ρ /s^-1"}, GridLines → None,
  Axes → None, PlotRange → Full, BaseStyle → {FontSize → 13},
  Frame → True, PlotTheme → "Monochrome", PlotLegends →
   {"num", "second L+K simpl", "sec L+K ext", "second L+K+R", "sec L+K extAGP"}]
a = 3
R1x = 1; R2x = 6;
w1x = 50;
k21exx = 100;
k31exx = 100;
k32exx = 0;
Pax = 0.9; Pbx = 0.05; Pcx = 0.05;
WBx = 300; WCx = -300;
a = -600; b = 600;
Plot[
  {uvw, Abs[R1rhothreelinearsecondorderReffCosSin[R1x, R2x, x, WBx, WCx, w1x, k21exx,
       k31exx, k32exx, Pax, Pbx, Pcx] - R1rhothreelinearexactr[R1x,
       R2x, x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx]],
   Abs[R1rhothreelinearsecondorderReffTrunc[R1x, R2x, x, WBx, WCx, w1x,
       k21exx, k31exx, k32exx, Pax, Pbx, Pcx] - R1rhothreelinearexactr[
       R1x, R2x, x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx]],
   Abs[R1rhothreelinearsecondorderReffLRK[R1x, R2x, x, WBx, WCx, w1x,
       k21exx, k31exx, k32exx, Pax, Pbx, Pcx] - R1rhothreelinearexactr[
       R1x, R2x, x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx]]},
  {x, a, b}, FrameLabel → {"ΔΩ /s^-1", "R1ρ error /s^-1"},
  GridLines → None,
```

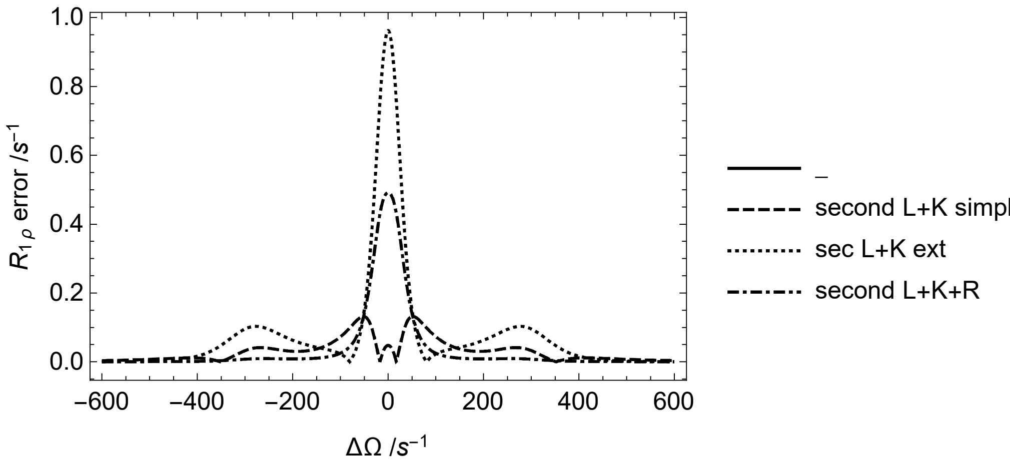
```
 Axes → None,
 PlotRange → Full,
 BaseStyle → {FontSize → 13},
 Frame → True, PlotTheme → "Monochrome",
 PlotLegends →
  {"_", "second L+K simpl", "sec L+K ext", "second L+K+R", "sec L+K extAGP"}]
R1rhothreelinearexactr[x, 200, -400, 50, 50, 10, 0, 0.7, 0.2, 0.1]
Plot[{R1rhothreelinearexactr[R1x, R2x, x, WBx, WCx, w1x, k21exx,
   k31exx, k32exx, Pax, Pbx, Pcx], R1rhothreelinearsecondorderReffCosSin[
   R1x, R2x, x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx],
  R1rhothreelinearsecondorderReffTrunc[R1x, R2x, x, WBx, WCx, w1x, k21exx,
   k31exx, k32exx, Pax, Pbx, Pcx], R1rhothreelinearsecondorderReffLRK[
   R1x, R2x, x, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx]},
 {x, a, b}, FrameLabel → {"ΔΩ /s^-1", "R1ρ /s^-1"}, GridLines → None,
 Axes → None, PlotRange → Full, BaseStyle → {FontSize → 13},
 Frame → True, PlotTheme → "Monochrome", PlotLegends →
  {"num", "second L+K simpl", "sec L+K ext", "second L+K+R", "sec L+K extAGP"}]
```



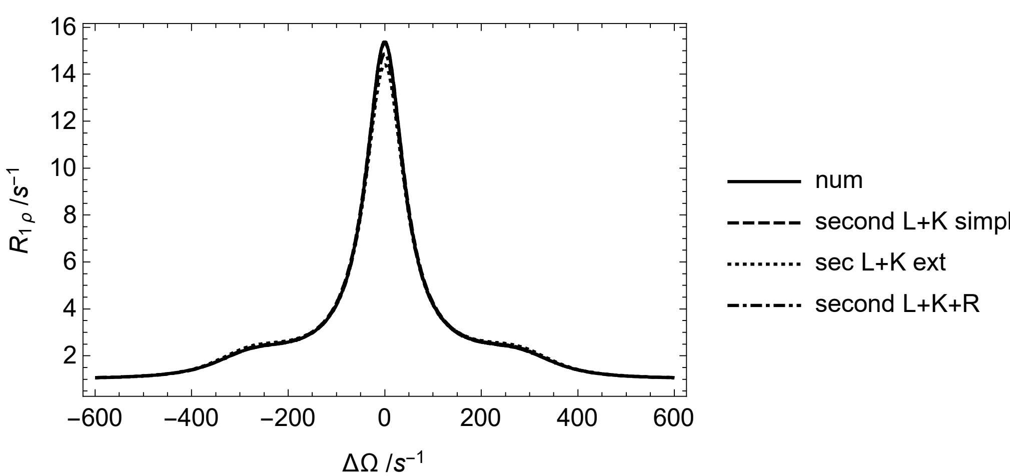

```
R1rhothreelinearexactr[x, 200, -400, 50, 50, 10, 0, 0.7, 0.2, 0.1]
```



3




```
R1rhothreelinearexactr[x, 200, -400, 50, 50, 10, 0, 0.7, 0.2, 0.1]
```



This is supplementary to Figure S4 - The contribution of the largest negative eigenvalue to the magnetization decay t = 0 s and ΔΩ = 0 s-1 is here calculated to be 83%, mostly due the presence of negative complex eigenvalues (using Eq. 6, similar to Fig. S1).

In[912]:=

```
thetax[WA_, WB_, WC_, w1_, Pa_, Pb_, Pc_] :=
 ArcSin[Sqrt[(w1^2) / (w1^2 + (Pa * WA + Pb * WB) ^2)]]
cossa[WA_, WB_, WC_, w1_, Pa_, Pb_, Pc_] := Pa * Cos[thetax[WA, WB, WC, w1, Pa, Pb, Pc]];
sinsa[WA_, WB_, WC_, w1_, Pa_, Pb_, Pc_] := Pa * Sin[thetax[WA, WB, WC, w1, Pa, Pb, Pc]];
cossb[WA_, WB_, WC_, w1_, Pa_, Pb_, Pc_] := Pb * Cos[thetax[WA, WB, WC, w1, Pa, Pb, Pc]];
sinsb[WA_, WB_, WC_, w1_, Pa_, Pb_, Pc_] := Pb * Sin[thetax[WA, WB, WC, w1, Pa, Pb, Pc]];
cossc[WA_, WB_, WC_, w1_, Pa_, Pb_, Pc_] := Pc * Cos[thetax[WA, WB, WC, w1, Pa, Pb, Pc]];
sinsc[WA_, WB_, WC_, w1_, Pa_, Pb_, Pc_] := Pc * Sin[thetax[WA, WB, WC, w1, Pa, Pb, Pc]];
lamf[R1_, R2_, DELTAO_, WB_, WC_, w1_,
   k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_] := Eigenvalues[
    (BigLtrr[R1, R2, DELTAO - Pb * WB - Pc * WC, WB + (DELTAO - Pb * WB - Pc * WC), WC +
        (DELTAO - Pb * WB - Pc * WC), w1] + Klinear[k21ex, k31ex, k32ex, Pa, Pb, Pc])] // N
uuf[R1_, R2_, DELTAO_, WB_, WC_, w1_, k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_] :=
 Eigenvectors[
    (BigLtrr[R1, R2, DELTAO - Pb * WB - Pc * WC, WB + (DELTAO - Pb * WB - Pc * WC), WC +
        (DELTAO - Pb * WB - Pc * WC), w1] + Klinear[k21ex, k31ex, k32ex, Pa, Pb, Pc])] // N
m0f[R1_, R2_, DELTAO_, WB_, WC_, w1_, k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_] :=
  {sinsa[DELTAO - Pb * WB - Pc * WC, WB + (DELTAO - Pb * WB - Pc * WC),
      WC + (DELTAO - Pb * WB - Pc * WC), w1, Pa, Pb, Pc], 0, cossa[DELTAO - Pb * WB - Pc * WC,
      WB + (DELTAO - Pb * WB - Pc * WC), WC + (DELTAO - Pb * WB - Pc * WC), w1, Pa, Pb, Pc],
     sinsb[DELTAO - Pb * WB - Pc * WC, WB + (DELTAO - Pb * WB - Pc * WC),
      WC + (DELTAO - Pb * WB - Pc * WC), w1, Pa, Pb, Pc], 0, cossb[DELTAO - Pb * WB - Pc * WC,
      WB + (DELTAO - Pb * WB - Pc * WC), WC + (DELTAO - Pb * WB - Pc * WC), w1, Pa, Pb, Pc],
     sinsc[DELTAO - Pb * WB - Pc * WC, WB + (DELTAO - Pb * WB - Pc * WC),
      WC + (DELTAO - Pb * WB - Pc * WC), w1, Pa, Pb, Pc], 0, cossc[DELTAO - Pb * WB - Pc * WC,
      WB + (DELTAO - Pb * WB - Pc * WC), WC + (DELTAO - Pb * WB - Pc * WC), w1, Pa, Pb, Pc]} // N;
mdf[R1_, R2_, DELTAO_, WB_, WC_, w1_, k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_] :=
  {Sin[thetax[DELTAO - Pb * WB - Pc * WC, WB + (DELTAO - Pb * WB - Pc * WC),
       WC + (DELTAO - Pb * WB - Pc * WC), w1, Pa, Pb, Pc]], 0,
     Cos[thetax[DELTAO - Pb * WB - Pc * WC, WB + (DELTAO - Pb * WB - Pc * WC),
       WC + (DELTAO - Pb * WB - Pc * WC), w1, Pa, Pb, Pc]],
     Sin[thetax[DELTAO - Pb * WB - Pc * WC, WB + (DELTAO - Pb * WB - Pc * WC),
       WC + (DELTAO - Pb * WB - Pc * WC), w1, Pa, Pb, Pc]], 0,
     Cos[thetax[DELTAO - Pb * WB - Pc * WC, WB + (DELTAO - Pb * WB - Pc * WC),
       WC + (DELTAO - Pb * WB - Pc * WC), w1, Pa, Pb, Pc]],
     Sin[thetax[DELTAO - Pb * WB - Pc * WC, WB + (DELTAO - Pb * WB - Pc * WC),
       WC + (DELTAO - Pb * WB - Pc * WC), w1, Pa, Pb, Pc]], 0,
     Cos[thetax[DELTAO - Pb * WB - Pc * WC, WB + (DELTAO - Pb * WB - Pc * WC),
       WC + (DELTAO - Pb * WB - Pc * WC), w1, Pa, Pb, Pc]]} // N;
umf[R1_, R2_, DELTAO_, WB_, WC_, w1_, k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_] :=
 Inverse[uuf[R1, R2, DELTAO, WB, WC, w1, k21ex, k31ex, k32ex, Pa, Pb, Pc]]
```

```
ftsinglefx[xx_, lo_, R1_, R2_, DELTAO_, WB_, WC_,
  w1_, k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_] :=
 Re[Sum[(uuf[R1, R2, DELTAO, WB, WC, w1, k21ex, k31ex, k32ex, Pa, Pb, Pc][[i]].
       mdf[R1, R2, DELTAO, WB, WC, w1, k21ex, k31ex, k32ex, Pa, Pb, Pc]) *
     (Transpose[umf[R1, R2, DELTAO, WB, WC, w1, k21ex, k31ex, k32ex, Pa, Pb, Pc]][[
        i]].m0f[R1, R2, DELTAO, WB, WC, w1, k21ex, k31ex, k32ex, Pa, Pb, Pc]) *
     Exp[lamf[R1, R2, DELTAO, WB, WC, w1, k21ex, k31ex, k32ex, Pa, Pb, Pc][[i]] xx],
    {i, lo, lo}] // N] *
  (Re[Sum[(uuf[R1, R2, DELTAO, WB, WC, w1, k21ex, k31ex, k32ex, Pa, Pb, Pc][[i]].
        mdf[R1, R2, DELTAO, WB, WC, w1, k21ex, k31ex, k32ex, Pa, Pb, Pc]) *
      (Transpose[umf[R1, R2, DELTAO, WB, WC, w1, k21ex, k31ex, k32ex, Pa, Pb, Pc]][[
         i]].m0f[R1, R2, DELTAO, WB, WC, w1, k21ex, k31ex, k32ex, Pa, Pb, Pc]) *
      Exp[lamf[R1, R2, DELTAO, WB, WC, w1, k21ex, k31ex, k32ex, Pa, Pb, Pc][[i]] 0],
     {i, lo, lo}] // N] / Abs[
    Re[Sum[(uuf[R1, R2, DELTAO, WB, WC, w1, k21ex, k31ex, k32ex, Pa, Pb, Pc][[i]].mdf[
          R1, R2, DELTAO, WB, WC, w1, k21ex, k31ex, k32ex, Pa, Pb, Pc]) * (Transpose[
           umf[R1, R2, DELTAO, WB, WC, w1, k21ex, k31ex, k32ex, Pa, Pb, Pc]][[i]].
         m0f[R1, R2, DELTAO, WB, WC, w1, k21ex, k31ex, k32ex, Pa, Pb, Pc]) *
       Exp[lamf[R1, R2, DELTAO, WB, WC, w1, k21ex, k31ex, k32ex, Pa, Pb, Pc][[i]] 0],
      {i, lo, lo}] // N]])
R1x =
 1;
R2x = 6;
w1x = 50;
k21exx = 100;
k31exx = 100;
k32exx = 0;
Pax = 0.33; Pbx = 0.33; Pcx = 0.34;
WBx = 300;
WCx = -300;
ftsinglefx[0, 1, R1x, R2x, 0, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx]
ftsinglefx[0, 2, R1x, R2x, 0, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx]
ftsinglefx[0, 3, R1x, R2x, 0, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx]
ftsinglefx[0, 4, R1x, R2x, 0, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx]
ftsinglefx[0, 5, R1x, R2x, 0, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx]
ftsinglefx[0, 6, R1x, R2x, 0, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx]
ftsinglefx[0, 7, R1x, R2x, 0, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx]
ftsinglefx[0, 8, R1x, R2x, 0, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx]
ftsinglefx[0, 9, R1x, R2x, 0, WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx]
maxt = 0.2
axx = 0
Plot[
 {Total[Map[Function[r, ftsinglefx[t, r, R1x, R2x, axx, WBx, WCx, w1x, k21exx, k31exx,
```

```
            k32exx, Pax, Pbx, Pcx]], {1, 2}]]},
    {t, 0, maxt}, PlotRange → Full, PlotTheme → "Monochrome",
    FrameLabel → {"t /s", "a₁·exp(-λ₁t)+a₂·exp(-λ₂t)"},
    GridLines → None, Axes → None,
    BaseStyle → {FontSize → 13}, Frame → True]
   Plot[{Total[Map[Function[r, ftsinglefx[t, r, R1x, R2x, axx, WBx,
            WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx]], {3, 4}]]},
    {t, 0, maxt}, PlotRange → Full, PlotTheme → "Monochrome",
    FrameLabel → {"t /s", "a₃·exp(-λ₃t)+a₄·exp(-λ₄t)"},
    GridLines → None, Axes → None,
    BaseStyle → {FontSize → 13}, Frame → True]
   Plot[{Total[Map[Function[r, ftsinglefx[t, r, R1x, R2x, axx, WBx,
            WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx]], {5, 6}]]},
    {t, 0, maxt}, PlotRange → Full, PlotTheme → "Monochrome",
    FrameLabel → {"t /s", "a₅·exp(-λ₅t)+a₆·exp(-λ₆t)"},
    GridLines → None, Axes → None,
    BaseStyle → {FontSize → 13}, Frame → True]
   Plot[{Total[Map[Function[r, ftsinglefx[t, r, R1x, R2x, axx,
            WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx]], {7}]]},
    {t, 0, maxt}, PlotRange → Full, PlotTheme → "Monochrome",
    FrameLabel → {"t /s", "a₇·exp(-λ₇t)"}, GridLines → None,
    Axes → None, BaseStyle → {FontSize → 13}, Frame → True]
   Plot[{Total[Map[Function[r, ftsinglefx[t, r, R1x, R2x, axx,
            WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx]], {8}]]},
    {t, 0, maxt}, PlotRange → Full, PlotTheme → "Monochrome",
    FrameLabel → {"t /s", "a₈·exp(-λ₈t)"}, GridLines → None,
    Axes → None, BaseStyle → {FontSize → 13}, Frame → True]
   Plot[{Total[Map[Function[r, ftsinglefx[t, r, R1x, R2x, axx,
            WBx, WCx, w1x, k21exx, k31exx, k32exx, Pax, Pbx, Pcx]], {9}]]},
    {t, 0, maxt}, PlotRange → Full, PlotTheme → "Monochrome",
    FrameLabel → {"t /s", "a₉·exp(-λ₉t)"}, GridLines → None,
    Axes → None, BaseStyle → {FontSize → 13}, Frame → True]
```

```
Out[926]= 0.0213355

Out[927]= 0.0213355

Out[928]= 0.0521936

Out[929]= 0.0521936

Out[930]= 0.018829

Out[931]= 0.018829

Out[932]= 0.046271
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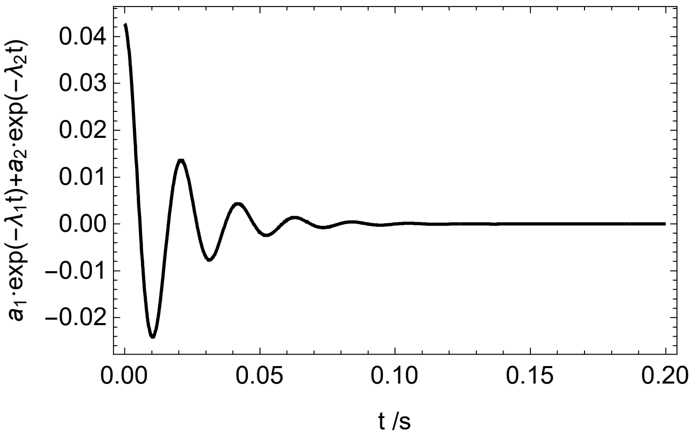
Out[933]= 0.0114974

Out[934]= 0.832831

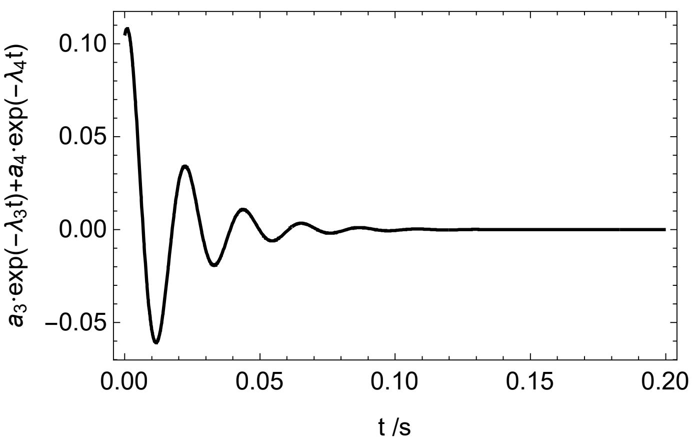
Out[935]= 0.2

Out[936]= 0

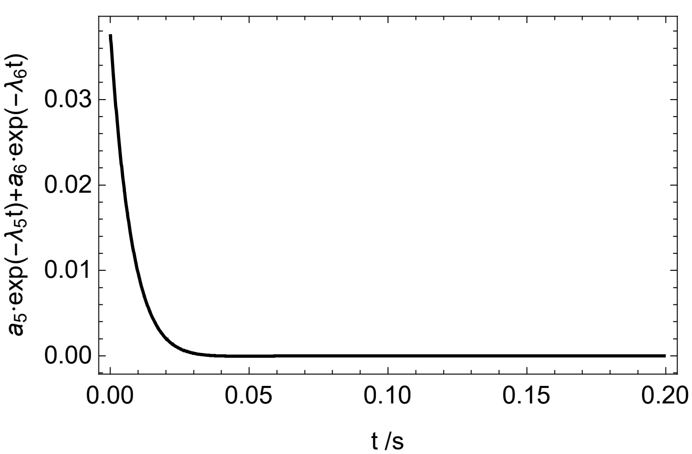
Out[937]=



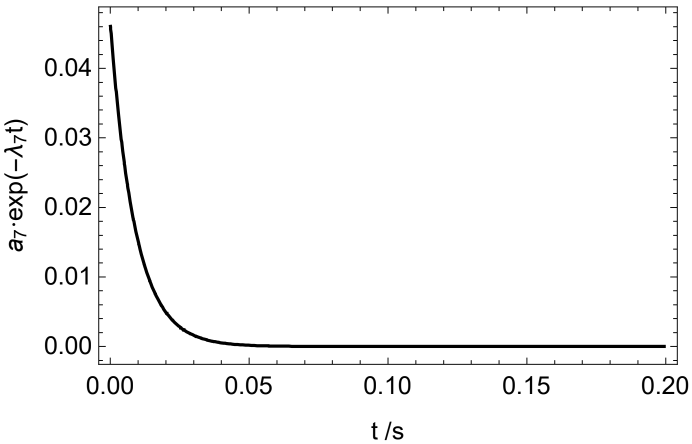
Out[938]=



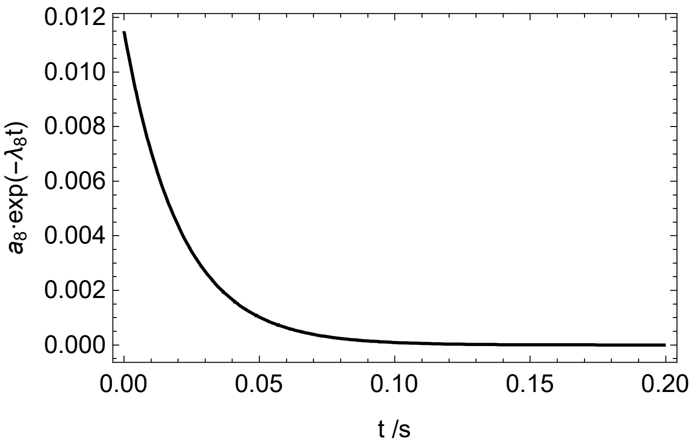
Out[939]=



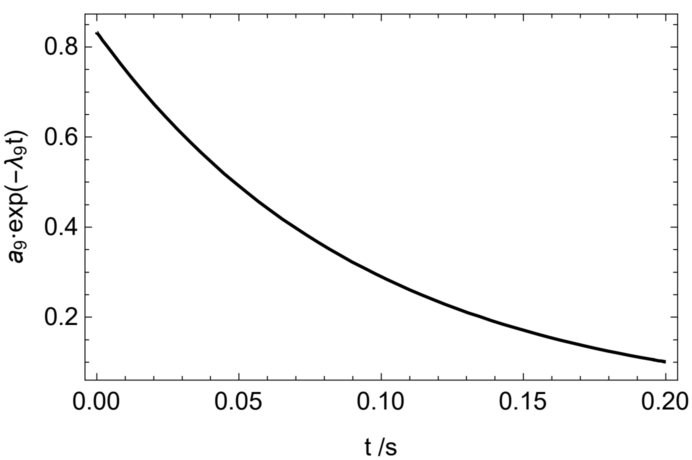
Out[940]=



Out[941]=



Out[942]=



This defines some L, I, rate constants - note that k21ex = k12ft + k21ft (and similar). Some rate constants differ only technically (using or not using dummy variables). Sinsq (theta) and the kinetic matrices for various four-site schemes are also defined in this block. There are also definitions for added L+K matrices.

In[943]:=
```
Off[General::luc]
I3 = IdentityMatrix[3];
LA = {{0, -WA, 0}, {WA, 0, -w1}, {0, w1, 0}};
LB = {{0, -WB, 0}, {WB, 0, -w1}, {0, w1, 0}};
LC = {{0, -WC, 0}, {WC, 0, -w1}, {0, w1, 0}};
LD = {{0, -WD, 0}, {WD, 0, -w1}, {0, w1, 0}};
MatrixForm[LA];
MatrixForm[LB];
MatrixForm[LC];
MatrixForm[LD];
BigL[WA_, WB_, WC_, WD_, w1_] = ArrayFlatten[{{LA, 0 I3, 0 I3, 0 I3},
    {0 I3, LB, 0 I3, 0 I3}, {0 I3, 0 I3, LC, 0 I3}, {0 I3, 0 I3, 0 I3, LD}}];
MatrixForm[BigL[WA, WB, WC, WD, w1]];
k34f[k21ex_, k31ex_, k41ex_, k43ex_, Pa_, Pb_, Pc_, Pd_] = k43ex / (1 + Pc / Pd);
k14f[k21ex_, k31ex_, k41ex_, k43ex_, Pa_, Pb_, Pc_, Pd_] = k41ex / (1 + Pa / Pd);
k13f[k21ex_, k31ex_, k41ex_, k43ex_, Pa_, Pb_, Pc_, Pd_] = k31ex / (1 + Pa / Pc);
k12f[k21ex_, k31ex_, k41ex_, k43ex_, Pa_, Pb_, Pc_, Pd_] = k21ex / (1 + Pa / Pb);
k21f[k21ex_, k31ex_, k41ex_, k43ex_, Pa_, Pb_, Pc_, Pd_] = k21ex - k21ex / (1 + Pa / Pb);
k43f[k21ex_, k31ex_, k41ex_, k43ex_, Pa_, Pb_, Pc_, Pd_] = k43ex - k43ex / (1 + Pc / Pd);
k41f[k21ex_, k31ex_, k41ex_, k43ex_, Pa_, Pb_, Pc_, Pd_] = k41ex - k41ex / (1 + Pa / Pd);
k31f[k21ex_, k31ex_, k41ex_, k43ex_, Pa_, Pb_, Pc_, Pd_] = k31ex - k31ex / (1 + Pa / Pc);
k14fst[k21ex_, k31ex_, k41ex_, Pa_, Pb_, Pc_, Pd_] = k41ex / (1 + Pa / Pd);
k13fst[k21ex_, k31ex_, k41ex_, Pa_, Pb_, Pc_, Pd_] = k31ex / (1 + Pa / Pc);
k12fst[k21ex_, k31ex_, k41ex_, Pa_, Pb_, Pc_, Pd_] = k21ex / (1 + Pa / Pb);
k21fst[k21ex_, k31ex_, k41ex_, Pa_, Pb_, Pc_, Pd_] = k21ex - k21ex / (1 + Pa / Pb);
k41fst[k21ex_, k31ex_, k41ex_, Pa_, Pb_, Pc_, Pd_] = k41ex - k41ex / (1 + Pa / Pd);
k31fst[k21ex_, k31ex_, k41ex_, Pa_, Pb_, Pc_, Pd_] = k31ex - k31ex / (1 + Pa / Pc);
Kkitematrix[k21ex_, k31ex_, k41ex_, k43ex_, Pa_, Pb_, Pc_, Pd_] = ArrayFlatten[
   {{(-k12f[k21ex, k31ex, k41ex, k43ex, Pa, Pb, Pc, Pd] - k13f[k21ex, k31ex, k41ex,
         k43ex, Pa, Pb, Pc, Pd] - k14f[k21ex, k31ex, k41ex, k43ex, Pa, Pb, Pc, Pd]) I3,
      k21f[k21ex, k31ex, k41ex, k43ex, Pa, Pb, Pc, Pd] I3,
      k31f[k21ex, k31ex, k41ex, k43ex, Pa, Pb, Pc, Pd] I3,
      k41f[k21ex, k31ex, k41ex, k43ex, Pa, Pb, Pc, Pd] I3},
     {k12f[k21ex, k31ex, k41ex, k43ex, Pa, Pb, Pc, Pd] I3,
      -k21f[k21ex, k31ex, k41ex, k43ex, Pa, Pb, Pc, Pd] I3, 0 I3, 0 I3},
     {k13f[k21ex, k31ex, k41ex, k43ex, Pa, Pb, Pc, Pd] I3, 0 I3,
      (-k31f[k21ex, k31ex, k41ex, k43ex, Pa, Pb, Pc, Pd] -
         k34f[k21ex, k31ex, k41ex, k43ex, Pa, Pb, Pc, Pd]) I3,
      k43f[k21ex, k31ex, k41ex, k43ex, Pa, Pb, Pc, Pd] I3},
```

```
      {k14f[k21ex, k31ex, k41ex, k43ex, Pa, Pb, Pc, Pd] I3, 0 I3,
       k34f[k21ex, k31ex, k41ex, k43ex, Pa, Pb, Pc, Pd] I3,
       (-k41f[k21ex, k31ex, k41ex, k43ex, Pa, Pb, Pc, Pd] -
          k43f[k21ex, k31ex, k41ex, k43ex, Pa, Pb, Pc, Pd]) I3}}];
MatrixForm[Kkitematrix[k21ex, k31ex, k41ex, k43ex, Pa, Pb, Pc, Pd]]
Kstarmatrix[k21ex_, k31ex_, k41ex_, Pa_, Pb_, Pc_, Pd_] =
  ArrayFlatten[{{(-k12fst[k21ex, k31ex, k41ex, Pa, Pb, Pc, Pd] - k13fst[k21ex, k31ex,
          k41ex, Pa, Pb, Pc, Pd] - k14fst[k21ex, k31ex, k41ex, Pa, Pb, Pc, Pd]) I3,
      k21fst[k21ex, k31ex, k41ex, Pa, Pb, Pc, Pd] I3, k31fst[k21ex, k31ex,
        k41ex, Pa, Pb, Pc, Pd] I3, k41fst[k21ex, k31ex, k41ex, Pa, Pb, Pc, Pd] I3},
     {k12fst[k21ex, k31ex, k41ex, Pa, Pb, Pc, Pd] I3,
      -k21fst[k21ex, k31ex, k41ex, Pa, Pb, Pc, Pd] I3, 0 I3, 0 I3},
     {k13fst[k21ex, k31ex, k41ex, Pa, Pb, Pc, Pd] I3, 0 I3,
      -k31fst[k21ex, k31ex, k41ex, Pa, Pb, Pc, Pd] I3, 0 I3},
     {k14fst[k21ex, k31ex, k41ex, Pa, Pb, Pc, Pd] I3, 0 I3, 0 I3,
      -k41fst[k21ex, k31ex, k41ex, Pa, Pb, Pc, Pd] I3}}];
MatrixForm[Kstarmatrix[k21ex, k31ex, k41ex, Pa, Pb, Pc, Pd]]
Klinearmatrix[k21ex_, k31ex_, k41ex_, k43ex_, PVa_, PVb_, PVc_, PVd_] :=
 ArrayFlatten[{{(-k12f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] -
        k13f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd]) I3,
     k21f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] I3,
     k31f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] I3, 0 I3},
    {k12f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] I3,
     -k21f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] I3, 0 I3, 0 I3},
    {k13f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] I3, 0 I3,
     -(k34f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] +
         k31f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd]) I3,
     k43f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] I3},
    {0 I3, 0 I3, k34f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] I3,
     -k43f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] I3}}]
MatrixForm[Klinearmatrix[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd]]

sinsqtheta[DELTAO_, WB_, WC_, WD_, w1_, Pa_, Pb_, Pc_, Pd_] :=
  (w1^2 / (w1^2 + ((DELTAO - Pb * WB - Pc * WC - Pd * WD) * Pa +
           (WB + (DELTAO - Pb * WB - Pc * WC - Pd * WD)) * Pb +
           (WC + (DELTAO - Pb * WB - Pc * WC - Pd * WD)) * Pc +
           (WD + (DELTAO - Pb * WB - Pc * WC - Pd * WD)) * Pd)^2));

kiteLK[DELTAO_, WB_, WC_, WD_, w1_, k21ex_, k31ex_, k41ex_, k43ex_, Pa_, Pb_, Pc_,
   Pd_] := BigL[DELTAO - Pb * WB - Pc * WC - Pd * WD, WB + (DELTAO - Pb * WB - Pc * WC - Pd * WD),
    WC + (DELTAO - Pb * WB - Pc * WC - Pd * WD), WD + (DELTAO - Pb * WB - Pc * WC - Pd * WD), w1] +
   Kkitematrix[k21ex, k31ex, k41ex, k43ex, Pa, Pb, Pc, Pd];
linearLK[DELTAO_, WB_, WC_, WD_, w1_, k21ex_, k31ex_,
```

```
k41ex_, k43ex_, PVa_, PVb_, PVc_, PVd_] :=
  BigL[DELTAO - PVb * WB - PVc * WC - PVd * WD, WB + (DELTAO - PVb * WB - PVc * WC - PVd * WD),
    WC + (DELTAO - PVb * WB - PVc * WC - PVd * WD), WD + (DELTAO - PVb * WB - PVc * WC - PVd * WD),
    w1] + Klinearmatrix[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd];
starlk[DELTAO_, WB_, WC_, WD_, w1_, k21ex_, k31ex_, k41ex_, Pa_, Pb_, Pc_, Pd_] :=
  BigL[DELTAO - Pb * WB - Pc * WC - Pd * WD, WB + (DELTAO - Pb * WB - Pc * WC - Pd * WD),
    WC + (DELTAO - Pb * WB - Pc * WC - Pd * WD), WD + (DELTAO - Pb * WB - Pc * WC - Pd * WD), w1] +
   Kstarmatrix[k21ex, k31ex, k41ex, Pa, Pb, Pc, Pd];
```

Out[970]//MatrixForm=

$$
\begin{pmatrix}
-\frac{k21ex}{1+\frac{Pa}{Pb}}-\frac{k31ex}{1+\frac{Pa}{Pc}}-\frac{k41ex}{1+\frac{Pa}{Pd}} & 0 & 0 & k21ex-\frac{k21ex}{1+\frac{Pa}{Pb}} & 0 \\
0 & -\frac{k21ex}{1+\frac{Pa}{Pb}}-\frac{k31ex}{1+\frac{Pa}{Pc}}-\frac{k41ex}{1+\frac{Pa}{Pd}} & 0 & 0 & k21ex-\frac{k21ex}{1+\frac{Pa}{Pb}} \\
0 & 0 & -\frac{k21ex}{1+\frac{Pa}{Pb}}-\frac{k31ex}{1+\frac{Pa}{Pc}}-\frac{k41ex}{1+\frac{Pa}{Pd}} & 0 & 0 \\
\frac{k21ex}{1+\frac{Pa}{Pb}} & 0 & 0 & -k21ex+\frac{k21ex}{1+\frac{Pa}{Pb}} & 0 \\
0 & \frac{k21ex}{1+\frac{Pa}{Pb}} & 0 & 0 & -k21ex+\frac{k21ex}{1+\frac{Pa}{Pb}} \\
0 & 0 & \frac{k21ex}{1+\frac{Pa}{Pb}} & 0 & 0 \\
\frac{k31ex}{1+\frac{Pa}{Pc}} & 0 & 0 & 0 & 0 \\
0 & \frac{k31ex}{1+\frac{Pa}{Pc}} & 0 & 0 & 0 \\
0 & 0 & \frac{k31ex}{1+\frac{Pa}{Pc}} & 0 & 0 \\
\frac{k41ex}{1+\frac{Pa}{Pd}} & 0 & 0 & 0 & 0 \\
0 & \frac{k41ex}{1+\frac{Pa}{Pd}} & 0 & 0 & 0 \\
0 & 0 & \frac{k41ex}{1+\frac{Pa}{Pd}} & 0 & 0
\end{pmatrix}
$$

Out[972]//MatrixForm=

$$\left(\begin{array}{cccccc}
-\frac{k21ex}{1+\frac{Pa}{Pb}}-\frac{k31ex}{1+\frac{Pa}{Pc}}-\frac{k41ex}{1+\frac{Pa}{Pd}} & 0 & 0 & k21ex-\frac{k21ex}{1+\frac{Pa}{Pb}} & 0 & \\
0 & -\frac{k21ex}{1+\frac{Pa}{Pb}}-\frac{k31ex}{1+\frac{Pa}{Pc}}-\frac{k41ex}{1+\frac{Pa}{Pd}} & 0 & 0 & k21ex-\frac{k21ex}{1+\frac{Pa}{Pb}} & \\
0 & 0 & -\frac{k21ex}{1+\frac{Pa}{Pb}}-\frac{k31ex}{1+\frac{Pa}{Pc}}-\frac{k41ex}{1+\frac{Pa}{Pd}} & 0 & 0 & \\
\frac{k21ex}{1+\frac{Pa}{Pb}} & 0 & 0 & -k21ex+\frac{k21ex}{1+\frac{Pa}{Pb}} & 0 & \\
0 & \frac{k21ex}{1+\frac{Pa}{Pb}} & 0 & 0 & -k21ex+\frac{k21ex}{1+\frac{Pa}{Pb}} & \\
0 & 0 & \frac{k21ex}{1+\frac{Pa}{Pb}} & 0 & 0 & - \\
\frac{k31ex}{1+\frac{Pa}{Pc}} & 0 & 0 & 0 & 0 & \\
0 & \frac{k31ex}{1+\frac{Pa}{Pc}} & 0 & 0 & 0 & \\
0 & 0 & \frac{k31ex}{1+\frac{Pa}{Pc}} & 0 & 0 & \\
\frac{k41ex}{1+\frac{Pa}{Pd}} & 0 & 0 & 0 & 0 & \\
0 & \frac{k41ex}{1+\frac{Pa}{Pd}} & 0 & 0 & 0 & \\
0 & 0 & \frac{k41ex}{1+\frac{Pa}{Pd}} & 0 & 0 &
\end{array}\right.$$

Out[974]//MatrixForm=

$$\left(\begin{array}{ccccccc}
-\frac{k21ex}{1+\frac{PVa}{PVb}}-\frac{k31ex}{1+\frac{PVa}{PVc}} & 0 & 0 & k21ex-\frac{k21ex}{1+\frac{PVa}{PVb}} & 0 & 0 & k\dots \\
0 & -\frac{k21ex}{1+\frac{PVa}{PVb}}-\frac{k31ex}{1+\frac{PVa}{PVc}} & 0 & 0 & k21ex-\frac{k21ex}{1+\frac{PVa}{PVb}} & 0 & \\
0 & 0 & -\frac{k21ex}{1+\frac{PVa}{PVb}}-\frac{k31ex}{1+\frac{PVa}{PVc}} & 0 & 0 & k21ex-\frac{k21ex}{1+\frac{PVa}{PVb}} & \\
\frac{k21ex}{1+\frac{PVa}{PVb}} & 0 & 0 & -k21ex+\frac{k21ex}{1+\frac{PVa}{PVb}} & 0 & 0 & \\
0 & \frac{k21ex}{1+\frac{PVa}{PVb}} & 0 & 0 & -k21ex+\frac{k21ex}{1+\frac{PVa}{PVb}} & 0 & \\
0 & 0 & \frac{k21ex}{1+\frac{PVa}{PVb}} & 0 & 0 & -k21ex+\frac{k21ex}{1+\frac{PVa}{PVb}} & \\
\frac{k31ex}{1+\frac{PVa}{PVc}} & 0 & 0 & 0 & 0 & 0 & -k31e\dots \\
0 & \frac{k31ex}{1+\frac{PVa}{PVc}} & 0 & 0 & 0 & 0 & \\
0 & 0 & \frac{k31ex}{1+\frac{PVa}{PVc}} & 0 & 0 & 0 & \\
0 & 0 & 0 & 0 & 0 & 0 & \\
0 & 0 & 0 & 0 & 0 & 0 & \\
0 & 0 & 0 & 0 & 0 & 0 &
\end{array}\right.$$

These are matrices and definitions needed to calculate the second-order approximation for the four-site scheme (Eqs. S1-S5, Eq 43).

In[979]:=
```
LAx[DELTAO_, WB_, WC_, WD_, w1_, PVa_, PVb_, PVc_, PVd_] =
  {{0, -(DELTAO - PVb * WB - PVc * WC - PVd * WD), 0},
   {(DELTAO - PVb * WB - PVc * WC - PVd * WD), 0, -w1}, {0, w1, 0}}
LBx[DELTAO_, WB_, WC_, WD_, w1_, PVa_, PVb_, PVc_, PVd_] =
  {{0, -(WB + DELTAO - PVb * WB - PVc * WC - PVd * WD), 0},
```

```
  {WB + DELTAO - PVb * WB - PVc * WC - PVd * WD, 0, -w1}, {0, w1, 0}}
LCx[DELTAO_, WB_, WC_, WD_, w1_, PVa_, PVb_, PVc_, PVd_] =
 {{0, - (WC + DELTAO - PVb * WB - PVc * WC - PVd * WD), 0},
  {WC + DELTAO - PVb * WB - PVc * WC - PVd * WD, 0, -w1}, {0, w1, 0}}
LDx[DELTAO_, WB_, WC_, WD_, w1_, PVa_, PVb_, PVc_, PVd_] =
 {{0, - (WD + DELTAO - PVb * WB - PVc * WC - PVd * WD), 0},
  {WD + DELTAO - PVb * WB - PVc * WC - PVd * WD, 0, -w1}, {0, w1, 0}}
LAz[DELTAO_, WB_, WC_, WD_, w1_, PVa_, PVb_, PVc_, PVd_, k21ex_, k31ex_,
   k41ex_, k43ex_] := LAx[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd] -
   (k12f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] +
      k13f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd]) * I3;
LBz[DELTAO_, WB_, WC_, WD_, w1_, PVa_, PVb_, PVc_, PVd_, k21ex_, k31ex_,
   k41ex_, k43ex_] := LBx[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd] -
   k21f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] * I3;
LCz[DELTAO_, WB_, WC_, WD_, w1_, PVa_, PVb_, PVc_, PVd_, k21ex_, k31ex_,
   k41ex_, k43ex_] := LCx[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd] -
   (k31f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] +
      k34f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd]) * I3;
LDz[DELTAO_, WB_, WC_, WD_, w1_, PVa_, PVb_, PVc_, PVd_, k21ex_, k31ex_,
   k41ex_, k43ex_] := LDx[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd] -
   k43f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] * I3;

XmatF[DELTAO_, WB_, WC_, WD_, w1_,
   PVa_, PVb_, PVc_, PVd_, k21ex_, k31ex_, k41ex_, k43ex_] :=
  (LBz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex].
     LAz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex].
     LCz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex]) +
   (LBz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex].
     LAz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex].
     LDz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex]) +
   LBz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex].
    LCz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex].
    LDz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex] +
   LAz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex].
    LCz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex].
    LDz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex] -
   (k13f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] * k31f[k21ex, k31ex, k41ex,
       k43ex, PVa, PVb, PVc, PVd] * I3 + k34f[k21ex, k31ex, k41ex, k43ex, PVa, PVb,
       PVc, PVd] * k43f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] * I3).
    LBz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex] -
   (k34f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] *
      k43f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] * I3).
    LAz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex] -
```

```
    (k12f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] *
       k21f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] * I3).
     LCz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex] -
    (k12f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] * k21f[k21ex, k31ex, k41ex,
          k43ex, PVa, PVb, PVc, PVd] * I3 + k13f[k21ex, k31ex, k41ex, k43ex, PVa, PVb,
          PVc, PVd] * k31f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] * I3).
     LDz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex];
YmatF[DELTAO_, WB_, WC_, WD_, w1_, PVa_, PVb_, PVc_, PVd_,
    k21ex_, k31ex_, k41ex_, k43ex_] :=
  LAz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex].
     LBz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex] +
    LAz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex].
     LCz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex] +
    LAz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex].
     LDz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex] +
    LBz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex].
     LCz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex] +
    LBz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex].
     LDz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex] +
    LCz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex].
     LDz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex] -
    k12f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] *
     k21f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] * I3 -
    k13f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] *
     k31f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] * I3 -
    k34f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] *
     k43f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] * I3;
ZmatF[DELTAO_, WB_, WC_, WD_, w1_, PVa_, PVb_, PVc_, PVd_,
    k21ex_, k31ex_, k41ex_, k43ex_] :=
   (LBz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex].
      LAz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex].
      LCz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex].
      LDz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex]) -
    (k34f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] *
       k43f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] * I3).
     LBz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex].
     LAz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex] -
    (k13f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] *
       k31f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] * I3).
     LBz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex].
     LDz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex] -
    (k12f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] *
       k21f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] * I3).
```

```
LCz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex].
LDz[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex] +
(k12f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] *
  k21f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] *
  k34f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] *
  k43f[k21ex, k31ex, k41ex, k43ex, PVa, PVb, PVc, PVd] * I3);
```

```
Out[979]= {{0, -DELTAO + PVb WB + PVc WC + PVd WD, 0},
  {DELTAO - PVb WB - PVc WC - PVd WD, 0, -w1}, {0, w1, 0}}

Out[980]= {{0, -DELTAO - WB + PVb WB + PVc WC + PVd WD, 0},
  {DELTAO + WB - PVb WB - PVc WC - PVd WD, 0, -w1}, {0, w1, 0}}

Out[981]= {{0, -DELTAO + PVb WB - WC + PVc WC + PVd WD, 0},
  {DELTAO - PVb WB + WC - PVc WC - PVd WD, 0, -w1}, {0, w1, 0}}

Out[982]= {{0, -DELTAO + PVb WB + PVc WC - WD + PVd WD, 0},
  {DELTAO - PVb WB - PVc WC + WD - PVd WD, 0, -w1}, {0, w1, 0}}
```

These are definitions which are needed to calculated the Woodbury approximation for the 4 - site kite scheme (Eq. 53)

In[990]:=
```
Umat = ArrayFlatten[{{-I3}, {0 I3}, {0 I3}, {I3}}];
MatrixForm[Umat]
Vmat[k21ex_, k31ex_, k41ex_, k43ex_, Pa_, Pb_, Pc_, Pd_] :=
  ArrayFlatten[{{k14f[k21ex, k31ex, k41ex, k43ex, Pa, Pb, Pc, Pd] I3,
     0 I3, 0 I3, -k41f[k21ex, k31ex, k41ex, k43ex, Pa, Pb, Pc, Pd] I3}}];
InvLK[DELTAO_, WB_, WC_, WD_, w1_, k21ex_, k31ex_, k41ex_,
   k43ex_, Pa_, Pb_, Pc_, Pd_] :=
  Inverse[BigL[DELTAO - Pb * WB - Pc * WC - Pd * WD, WB + (DELTAO - Pb * WB - Pc * WC - Pd * WD),
     WC + (DELTAO - Pb * WB - Pc * WC - Pd * WD), WD + (DELTAO - Pb * WB - Pc * WC - Pd * WD), w1] +
    Klinearmatrix[k21ex, k31ex, k41ex, k43ex, Pa, Pb, Pc, Pd]];
InvLKsq[DELTAO_, WB_, WC_, WD_, w1_, k21ex_, k31ex_, k41ex_, k43ex_, Pa_, Pb_,
  Pc_, Pd_] := InvLK[DELTAO, WB, WC, WD, w1, k21ex, k31ex, k41ex, k43ex, Pa, Pb, Pc, Pd].
  InvLK[DELTAO, WB, WC, WD, w1, k21ex, k31ex, k41ex, k43ex, Pa, Pb, Pc, Pd]
TrZVersion1[DELTAO_, WB_, WC_, WD_, w1_, k21ex_, k31ex_, k41ex_, k43ex_,
  Pa_, Pb_, Pc_, Pd_] := Tr[(Vmat[k21ex, k31ex, k41ex, k43ex, Pa, Pb, Pc, Pd].
     InvLKsq[DELTAO, WB, WC, WD, w1, k21ex, k31ex, k41ex, k43ex, Pa, Pb, Pc, Pd].Umat).
   Inverse[I3 + Vmat[k21ex, k31ex, k41ex, k43ex, Pa, Pb, Pc, Pd].
      InvLK[DELTAO, WB, WC, WD, w1, k21ex, k31ex, k41ex, k43ex, Pa, Pb, Pc, Pd].Umat]]
```

Out[991]//MatrixForm=

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

These are all numerical calculation and all approximations for all three considered four - site - schemes.

In[996]:=
```
fourlinearexact[DELTAO_, WB_, WC_, WD_,
   w1_, k21ex_, k31ex_, k41ex_, k43ex_, Pa_, Pb_, Pc_, Pd_] :=
  -N[Re[Eigenvalues[linearLK[DELTAO, WB, WC, WD, w1, k21ex, k31ex, k41ex, k43ex, Pa,
        Pb, Pc, Pd]]]][[12]] / sinsqtheta[DELTAO, WB, WC, WD, w1, Pa, Pb, Pc, Pd];
fourlinearfirstorder[DELTAO_, WB_, WC_, WD_, w1_, k21ex_, k31ex_,
   k41ex_, k43ex_, Pa_, Pb_, Pc_, Pd_] :=
  - (1 / Tr[Inverse[linearLK[DELTAO, WB, WC, WD, w1,
        k21ex, k31ex, k41ex, k43ex, Pa, Pb, Pc, Pd]]]) /
   sinsqtheta[DELTAO, WB, WC, WD, w1, Pa, Pb, Pc, Pd];
fourlinearsecondorder[DELTAO_, WB_, WC_, WD_, w1_, k21ex_,
   k31ex_, k41ex_, k43ex_, PVa_, PVb_, PVc_, PVd_] :=
  - (1 / (Tr[Inverse[ZmatF[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc,
          PVd, k21ex, k31ex, k41ex, k43ex]].XmatF[DELTAO, WB, WC,
```

```
            WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex]] -
        Tr[Inverse[ZmatF[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex,
              k31ex, k41ex, k43ex]].YmatF[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd,
             k21ex, k31ex, k41ex, k43ex] + Minors[Inverse[ZmatF[DELTAO, WB, WC,
               WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex]].XmatF[DELTAO,
              WB, WC, WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex]]] /
         Tr[Inverse[ZmatF[DELTAO, WB, WC, WD, w1, PVa, PVb, PVc, PVd,
             k21ex, k31ex, k41ex, k43ex]].XmatF[DELTAO, WB, WC,
            WD, w1, PVa, PVb, PVc, PVd, k21ex, k31ex, k41ex, k43ex]])) /
   sinsqtheta[DELTAO, WB, WC, WD, w1, PVa, PVb,
    PVc,
    PVd];

fourkiteexact[DELTAO_, WB_, WC_, WD_, w1_,
  k21ex_, k31ex_, k41ex_, k43ex_, Pa_, Pb_, Pc_, Pd_] :=
 -N[Re[Eigenvalues[kiteLK[DELTAO, WB, WC, WD, w1, k21ex, k31ex, k41ex, k43ex, Pa,
        Pb, Pc, Pd]]][[12]]] / sinsqtheta[DELTAO, WB, WC, WD, w1, Pa, Pb, Pc, Pd]
fourkitefirstorder[DELTAO_, WB_, WC_, WD_, w1_, k21ex_, k31ex_,
   k41ex_, k43ex_, Pa_, Pb_, Pc_, Pd_] :=
  - (1 / Tr[Inverse[kiteLK[DELTAO, WB, WC, WD, w1, k21ex, k31ex, k41ex, k43ex, Pa,
         Pb, Pc, Pd]]]) / sinsqtheta[DELTAO, WB, WC, WD, w1, Pa, Pb, Pc, Pd];
fourkitewoodbury[DELTAO_, WB_, WC_, WD_, w1_, k21ex_, k31ex_,
  k41ex_, k43ex_, Pa_, Pb_, Pc_, Pd_] :=
 fourlinearsecondorder[DELTAO, WB, WC, WD, w1, k21ex, k31ex, k41ex, k43ex,
   Pa, Pb, Pc, Pd] * (1 / (1 + sinsqtheta[DELTAO, WB, WC, WD, w1, Pa, Pb, Pc, Pd] *
       fourlinearfirstorder[DELTAO, WB, WC, WD, w1, k21ex, k31ex,
        k41ex, k43ex, Pa, Pb, Pc, Pd] * TrZVersion1[DELTAO, WB,
        WC, WD, w1, k21ex, k31ex, k41ex, k43ex, Pa, Pb, Pc, Pd]))

fourstarexact[DELTAO_, WB_, WC_, WD_,
   w1_, k21ex_, k31ex_, k41ex_, k43ex_, Pa_, Pb_, Pc_, Pd_] :=
  -N[Re[Eigenvalues[starlk[DELTAO, WB, WC, WD, w1, k21ex, k31ex, k41ex, Pa, Pb,
         Pc, Pd]]]][[12]] / sinsqtheta[DELTAO, WB, WC, WD, w1, Pa, Pb, Pc, Pd];
fourstarfirstorder[DELTAO_, WB_, WC_, WD_, w1_, k21ex_, k31ex_,
   k41ex_, k43ex_, Pa_, Pb_, Pc_, Pd_] :=
  - (1 / Tr[Inverse[starlk[DELTAO, WB, WC, WD, w1, k21ex, k31ex, k41ex, Pa, Pb,
         Pc, Pd]]]) / sinsqtheta[DELTAO, WB, WC, WD, w1, Pa, Pb, Pc, Pd];
```

In this additional section, the numerical solution for three-state linear exchange is calculated (see also script for three sites). One of the figure demonstrates how to use pseudo-sites comparing a 4-site kite-scheme with a pseudo-site with a linear 3-site scheme.

In[1004]:=
```
k23ft[k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_] = k32ex / (1 + Pb / Pc);
k13ft[k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_] = k31ex / (1 + Pa / Pc);
k12ft[k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_] = k21ex / (1 + Pa / Pb);
k32ft[k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_] = k32ex - k32ex / (1 + Pb / Pc);
k31ft[k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_] = k31ex - k31ex / (1 + Pa / Pc);
k21ft[k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_] = k21ex - k21ex / (1 + Pa / Pb);
Klinearthree[k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_] = ArrayFlatten[
   {{(-k12ft[k21ex, k31ex, k32ex, Pa, Pb, Pc] - k13ft[k21ex, k31ex, k32ex, Pa, Pb, Pc])
       I3, k21ft[k21ex, k31ex, k32ex, Pa, Pb, Pc] I3,
      k31ft[k21ex, k31ex, k32ex, Pa, Pb, Pc] I3},
     {k12ft[k21ex, k31ex, k32ex, Pa, Pb, Pc] I3,
      -k21ft[k21ex, k31ex, k32ex, Pa, Pb, Pc] I3, 0 I3},
     {k13ft[k21ex, k31ex, k32ex, Pa, Pb, Pc] I3, 0 I3,
      -k31ft[k21ex, k31ex, k32ex, Pa, Pb, Pc] I3}}];
MatrixForm[Klinearthree[k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_]]
BigLthree[WA_, WB_, WC_, w1_] =
  ArrayFlatten[{{LA, 0 I3, 0 I3}, {0 I3, LB, 0 I3}, {0 I3, 0 I3, LC}}];
sinsqthetathree[DELTAO_, WB_, WC_, w1_, Pa_, Pb_, Pc_] :=
 (w1^2 / (w1^2 + ((DELTAO - Pb * WB - Pc * WC) * Pa +
        (WB + (DELTAO - Pb * WB - Pc * WC)) * Pb + (WC + (DELTAO - Pb * WB - Pc * WC)) * Pc)^2))
threelinearexact[DELTAO_, WB_, WC_, w1_, k21ex_, k31ex_, k32ex_, Pa_, Pb_, Pc_] :=
 -N[Re[Eigenvalues[Klinearthree[k21ex, k31ex, k32ex, Pa, Pb, Pc] +
        BigLthree[DELTAO - Pb * WB - Pc * WC, WB + (DELTAO - Pb * WB - Pc * WC),
         WC + (DELTAO - Pb * WB - Pc * WC), w1]]]][[9]] /
  sinsqthetathree[DELTAO, WB, WC, w1, Pa, Pb, Pc]
```

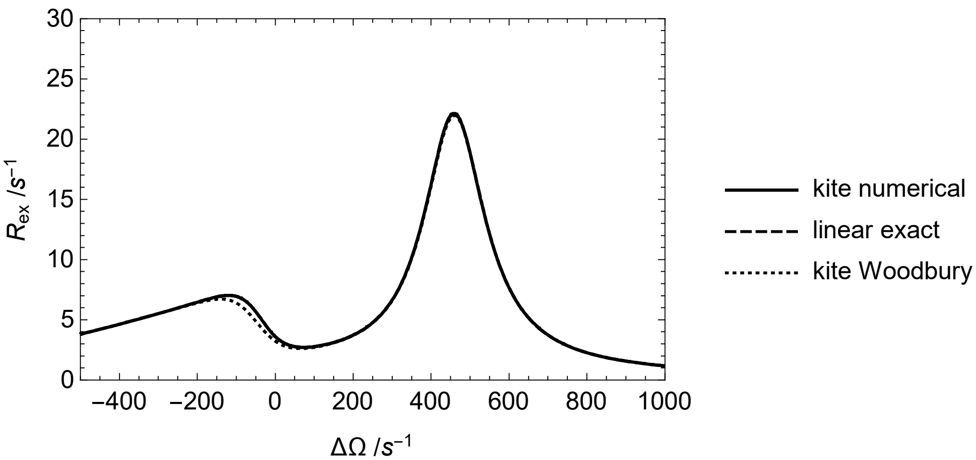
Out[1011]//MatrixForm=

$-\frac{k21ex\_}{1+\frac{Pa\_}{Pb\_}}-\frac{k31ex\_}{1+\frac{Pa\_}{Pc\_}}$	0	0	$k21ex\_-\frac{k21ex\_}{1+\frac{Pa\_}{Pb\_}}$	0	0
0	$-\frac{k21ex\_}{1+\frac{Pa\_}{Pb\_}}-\frac{k31ex\_}{1+\frac{Pa\_}{Pc\_}}$	0	0	$k21ex\_-\frac{k21ex\_}{1+\frac{Pa\_}{Pb\_}}$	0
0	0	$-\frac{k21ex\_}{1+\frac{Pa\_}{Pb\_}}-\frac{k31ex\_}{1+\frac{Pa\_}{Pc\_}}$	0	0	k21ex_ - k2…
$\frac{k21ex\_}{1+\frac{Pa\_}{Pb\_}}$	0	0	$-k21ex\_+\frac{k21ex\_}{1+\frac{Pa\_}{Pb\_}}$	0	0
0	$\frac{k21ex\_}{1+\frac{Pa\_}{Pb\_}}$	0	0	$-k21ex\_+\frac{k21ex\_}{1+\frac{Pa\_}{Pb\_}}$	0
0	0	$\frac{k21ex\_}{1+\frac{Pa\_}{Pb\_}}$	0	0	-k21ex_ + k2…
$\frac{k31ex\_}{1+\frac{Pa\_}{Pc\_}}$	0	0	0	0	0
0	$\frac{k31ex\_}{1+\frac{Pa\_}{Pc\_}}$	0	0	0	0
0	0	$\frac{k31ex\_}{1+\frac{Pa\_}{Pc\_}}$	0	0	0

The following sections plot Figures S7, S6, 4 and 4(insets). Refer to paper for details.

In[1015]:=
```
Plot[{fourkiteexact[x, -500, 200, 0, 100, 10, 500, 10 000, 10 000, 0.84999, 0.1, 0.05,
    0.00001], threelinearexact[x, -500, 200, 100, 10, 500, 1000, 0.85, 0.1, 0.05],
   fourkitewoodbury[x, -500, 200, 0, 100, 10, 500, 10 000, 1000,
    0.84999, 0.1, 0.05, 0.0001]}, {x, -500, 1000}, GridLines → None,
  FrameLabel → {"ΔΩ /s^-1", "R_ex /s^-1"}, PlotRange → {{-500, 1000}, {0, 30}},
  Axes → None, BaseStyle → {FontSize → 13}, Frame → True, PlotTheme → "Monochrome",
  PlotLegends → {"kite numerical", "linear exact", "kite Woodbury"}]
```

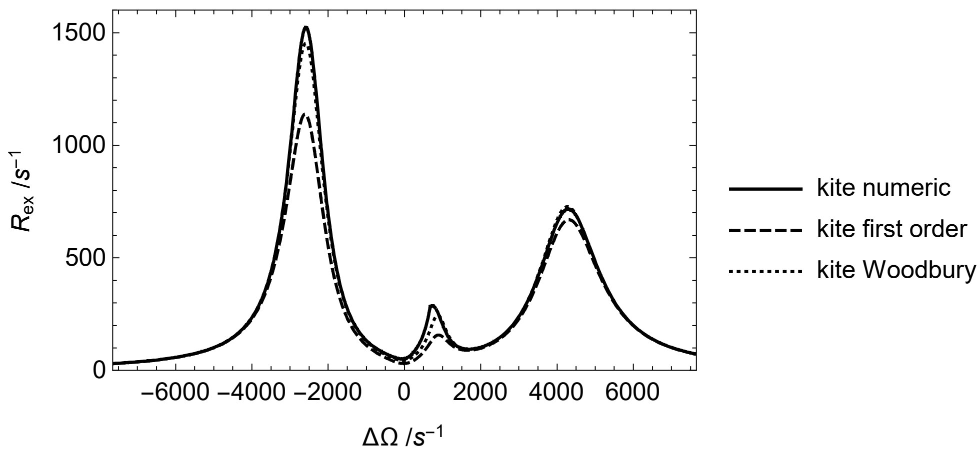
Out[1015]=



```
In[1016]:= a = 0.85; b = 0.7; d = 3; y = 350; f = 500; g = 1000; h = 500; kf = 1;  kg = 1;
  pax = 0.33
  Plot[{fourkiteexact[x, a * -1000, a * 3000, a * -5000, y, b * 200, b * h, b * f, kg * b * g,
      pax, 10 * (1 - pax) / 16 + (1 - kf) * 1 * (1 - pax) / 16, 5 * (1 - pax) / 16, kf * (1 - pax) / 16],
     fourkitefirstorder[x, a * -1000, a * 3000, a * -5000, y, b * 200, b * h, b * f, kg * b * g,
      pax, 10 * (1 - pax) / 16 + (1 - kf) * 1 * (1 - pax) / 16, 5 * (1 - pax) / 16, kf * (1 - pax) / 16],
     fourkitewoodbury[x, a * -1000, a * 3000, a * -5000, y, b * 200, b * h, b * f, kg * b * g, pax,
      10 * (1 - pax) / 16 + (1 - kf) * 1 * (1 - pax) / 16, 5 * (1 - pax) / 16, kf * (1 - pax) / 16]},
   {x, -3000 * d * a, 3000 * d * a}, PlotRange → {{-3000 * d * a, 3000 * d * a}, {0, 1600}},
   GridLines → None, FrameLabel → {"ΔΩ  /s^-1", "R_ex  /s^-1"}, Axes → None,
   BaseStyle → {FontSize → 13}, Frame → True, PlotTheme → "Monochrome",
   PlotLegends → {"kite numeric", "kite first order", "kite Woodbury"}]
  a = 0.85; b = 0.7; d = 3; y = 350; f = 500; g = 1000; h = 500; kf = 1;  kg = 1;
  pax = 0.55
  Plot[{fourkiteexact[x, a * -1000, a * 3000, a * -5000, y, b * 200, b * h, b * f, kg * b * g,
      pax, 10 * (1 - pax) / 16 + (1 - kf) * 1 * (1 - pax) / 16, 5 * (1 - pax) / 16, kf * (1 - pax) / 16],
     fourkitefirstorder[x, a * -1000, a * 3000, a * -5000, y, b * 200, b * h, b * f, kg * b * g,
      pax, 10 * (1 - pax) / 16 + (1 - kf) * 1 * (1 - pax) / 16, 5 * (1 - pax) / 16, kf * (1 - pax) / 16],
     fourkitewoodbury[x, a * -1000, a * 3000, a * -5000, y, b * 200, b * h, b * f, kg * b * g, pax,
      10 * (1 - pax) / 16 + (1 - kf) * 1 * (1 - pax) / 16, 5 * (1 - pax) / 16, kf * (1 - pax) / 16]},
   {x, -3000 * d * a, 3000 * d * a}, PlotRange → {{-3000 * d * a, 3000 * d * a}, {0, 1400}},
   GridLines → None, FrameLabel → {"ΔΩ  /s^-1", "R_ex  /s^-1"}, Axes → None,
   BaseStyle → {FontSize → 13}, Frame → True, PlotTheme → "Monochrome",
   PlotLegends → {"kite numeric", "kite first order", "kite Woodbury"}]
  a = 0.85; b = 0.7; d = 3; y = 350; f = 500; g = 1000; h = 500; kf = 1;  kg = 1;
  pax = 0.88
  Plot[{fourkiteexact[x, a * -1000, a * 3000, a * -5000, y, b * 200, b * h, b * f, kg * b * g,
      pax, 10 * (1 - pax) / 16 + (1 - kf) * 1 * (1 - pax) / 16, 5 * (1 - pax) / 16, kf * (1 - pax) / 16],
     fourkitefirstorder[x, a * -1000, a * 3000, a * -5000, y, b * 200, b * h, b * f, kg * b * g,
      pax, 10 * (1 - pax) / 16 + (1 - kf) * 1 * (1 - pax) / 16, 5 * (1 - pax) / 16, kf * (1 - pax) / 16],
     fourkitewoodbury[x, a * -1000, a * 3000, a * -5000, y, b * 200, b * h, b * f, kg * b * g, pax,
      10 * (1 - pax) / 16 + (1 - kf) * 1 * (1 - pax) / 16, 5 * (1 - pax) / 16, kf * (1 - pax) / 16]},
   {x, -3000 * d * a, 3000 * d * a}, PlotRange → {{-3000 * d * a, 3000 * d * a}, {0, 400}},
   GridLines → None, FrameLabel → {"ΔΩ  /s^-1", "R_ex  /s^-1"}, Axes → None,
   BaseStyle → {FontSize → 13}, Frame → True, PlotTheme → "Monochrome",
   PlotLegends → {"kite numeric", "kite first order", "kite Woodbury"}]

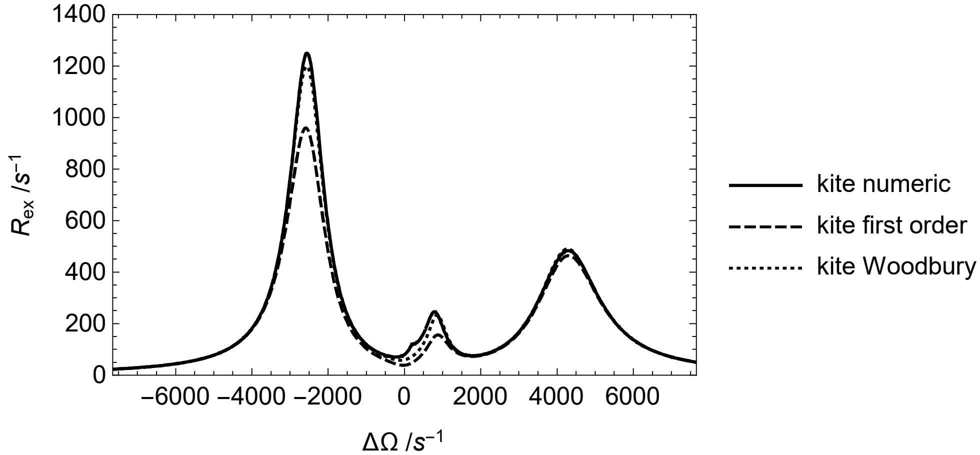
Out[1017]= 0.33
```

Out[1018]=



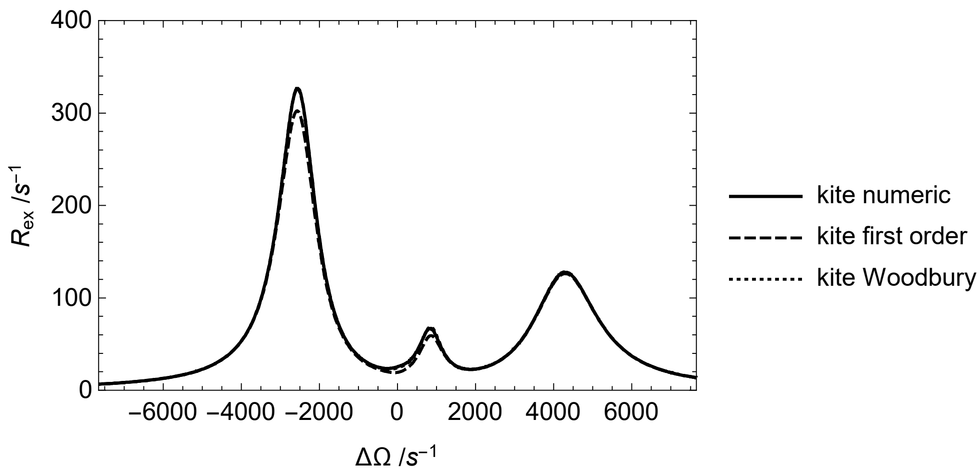
Out[1020]= 0.55

Out[1021]=



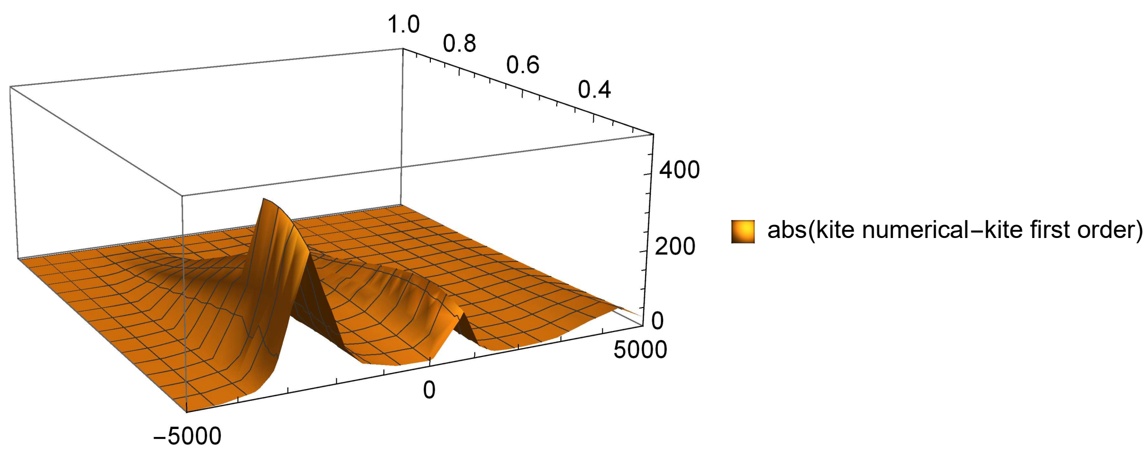
Out[1023]= 0.88

Out[1024]=

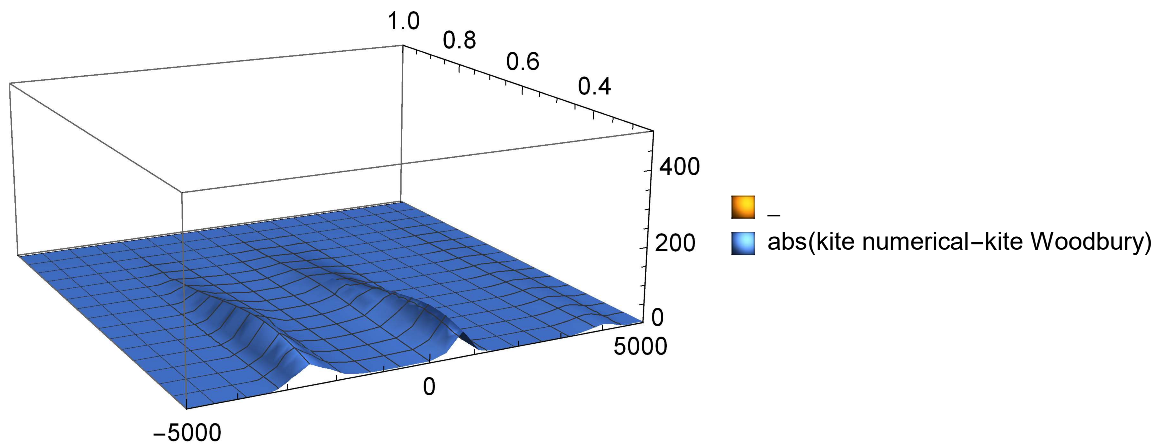


In[1025]:=
```
Plot3D[
 {Abs[fourkiteexact[x, a * -1000, a * 3000, a * -5000, y, b * 200, b * 500, b * 500, b * 1000,
     pax, 10 * (1 - pax) / 16, 5 * (1 - pax) / 16, 1 * (1 - pax) / 16] -
    fourkitefirstorder[x, a * -1000, a * 3000, a * -5000, y, b * 200, b * 500,
     b * 500, b * 1000, pax, 10 * (1 - pax) / 16, 5 * (1 - pax) / 16, 1 * (1 - pax) / 16]]},
 {x, -3000 * 2 * a, 3000 * 2 * a}, {pax, 0.2, 0.99}, AxesStyle → Directive[Black],
 PlotRange → {{-5000, 5000}, {0.25, 1}, {0, 500}},
 BaseStyle → {FontSize → 13, FontColor → Black},
 PlotLegends → {"abs(kite numerical-kite first order)"},
 ViewPoint → {-Pi / 2, -Pi, 1}]
Plot3D[{xx, Abs[fourkiteexact[x, a * -1000, a * 3000, a * -5000, y, b * 200, b * 500,
     b * 500, b * 1000, pax, 10 * (1 - pax) / 16, 5 * (1 - pax) / 16, 1 * (1 - pax) / 16] -
    fourkitewoodbury[x, a * -1000, a * 3000, a * -5000, y, b * 200, b * 500, b * 500,
     b * 1000, pax, 10 * (1 - pax) / 16, 5 * (1 - pax) / 16, 1 * (1 - pax) / 16]]},
 {x, -3000 * 2 * a, 3000 * 2 * a}, {pax, 0.2, 0.99},
 AxesStyle → Directive[Black],
 PlotRange → {{-5000, 5000}, {0.25, 1}, {0, 500}},
 BaseStyle → {FontSize → 13, FontColor → Black},
 PlotLegends → {"_", "abs(kite numerical-kite Woodbury)"},
 ViewPoint → {-Pi / 2, -Pi, 1}]
```

Out[1025]=



Out[1026]=



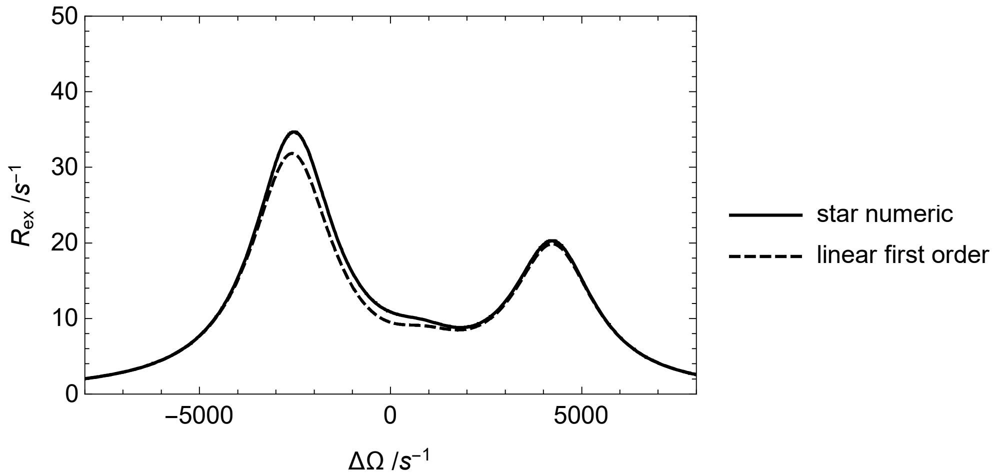
In[1027]:=

```
a = 0.9;
b = 0.05;
d = 3;
y = 50;
f = 500;
g = 1000;
h = 500;
w1x = 1250;
ran1 = 8000;
ran2 = 8000;
ran3 = 50;
Plot[{fourstarexact[x, -850, 2550, -4250, w1x, 140, 350,
    350, 700, 0.92, 0.05, 0.025, 0.005], fourstarfirstorder[x, -850,
    2550, -4250, w1x, 140, 350, 350, 700, 0.92, 0.05, 0.025, 0.005]},
  {x, -ran1, ran2}, PlotRange → {{-ran1, ran2}, {0, ran3}}, GridLines → None,
  FrameLabel → {"ΔΩ /s^-1", "R_ex /s^-1"}, Axes → None,
  BaseStyle → {FontSize → 13}, Frame → True, PlotTheme → "Monochrome",
  PlotLegends → {"star numeric", "linear first order"}]
Plot[{fourkiteexact[x, -850, 2550, -4250, w1x, 140, 350, 350, 700, 0.92,
    0.05, 0.025, 0.005], fourkitefirstorder[x, -850, 2550, -4250, w1x,
    140, 350, 350, 700, 0.92, 0.05, 0.025, 0.005], fourkitewoodbury[x,
    -850, 2550, -4250, w1x, 140, 350, 350, 700, 0.92, 0.05, 0.025, 0.005]},
  {x, -ran1, ran2}, PlotRange → {{-ran1, ran2}, {0, ran3}}, GridLines → None,
  FrameLabel → {"ΔΩ /s^-1", "R_ex /s^-1"}, Axes → None,
  BaseStyle → {FontSize → 13}, Frame → True, PlotTheme → "Monochrome",
  PlotLegends → {"kite numeric", "kite first order", "kite Woodbury"}]
Plot[{fourlinearexact[x, -850, 2550, -4250, w1x, 140, 350, 350, 700, 0.92,
    0.05, 0.025, 0.005], fourlinearfirstorder[x, -850, 2550, -4250, w1x,
    140, 350, 350, 700, 0.92, 0.05, 0.025, 0.005], fourlinearsecondorder[x,
    -850, 2550, -4250, w1x, 140, 350, 350, 700, 0.92, 0.05, 0.025, 0.005]},
  {x, -ran1, ran2}, PlotRange → {{-ran1, ran2}, {0, ran3}}, GridLines → None,
```

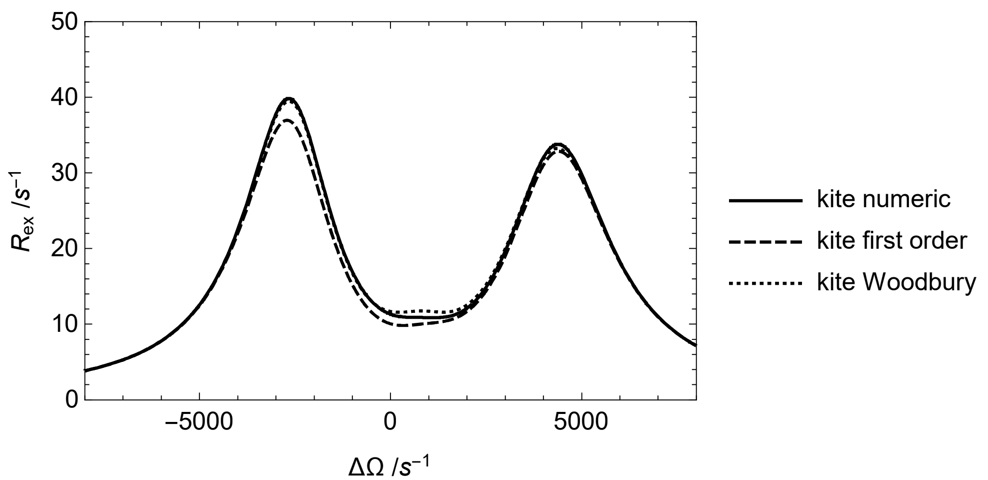
```
 FrameLabel → {"ΔΩ /s^-1", "R_ex /s^-1"}, Axes → None,
 BaseStyle → {FontSize → 13}, Frame → True, PlotTheme → "Monochrome",
 PlotLegends → {"linear numeric", "linear first order", "linear second order"}]
w1x = 350; ran1 = 8000; ran2 = 8000; ran3 = 250;
Plot[{fourstarexact[x, -850, 2550, -4250, w1x, 140, 350,
   350, 700, 0.92, 0.05, 0.025, 0.005], fourstarfirstorder[x, -850,
   2550, -4250, w1x, 140, 350, 350, 700, 0.92, 0.05, 0.025, 0.005]},
 {x, -ran1, ran2}, PlotRange → {{-ran1, ran2}, {0, ran3}}, GridLines → None,
 FrameLabel → {"ΔΩ /s^-1", "R_ex /s^-1"}, Axes → None,
 BaseStyle → {FontSize → 13}, Frame → True, PlotTheme → "Monochrome",
 PlotLegends → {"star numeric", "linear first order"}]
Plot[{fourkiteexact[x, -850, 2550, -4250, w1x, 140, 350, 350, 700, 0.92,
   0.05, 0.025, 0.005], fourkitefirstorder[x, -850, 2550, -4250, w1x,
   140, 350, 350, 700, 0.92, 0.05, 0.025, 0.005], fourkitewoodbury[x,
   -850, 2550, -4250, w1x, 140, 350, 350, 700, 0.92, 0.05, 0.025, 0.005]},
 {x, -ran1, ran2}, PlotRange → {{-ran1, ran2}, {0, ran3}}, GridLines → None,
 FrameLabel → {"ΔΩ /s^-1", "R_ex /s^-1"}, Axes → None,
 BaseStyle → {FontSize → 13}, Frame → True, PlotTheme → "Monochrome",
 PlotLegends → {"kite numeric", "kite first order", "kite Woodbury"}]
Plot[{fourlinearexact[x, -850, 2550, -4250, w1x, 140, 350, 350, 700, 0.92,
   0.05, 0.025, 0.005], fourlinearfirstorder[x, -850, 2550, -4250, w1x,
   140, 350, 350, 700, 0.92, 0.05, 0.025, 0.005], fourlinearsecondorder[x,
   -850, 2550, -4250, w1x, 140, 350, 350, 700, 0.92, 0.05, 0.025, 0.005]},
 {x, -ran1, ran2}, PlotRange → {{-ran1, ran2}, {0, ran3}}, GridLines → None,
 FrameLabel → {"ΔΩ /s^-1", "R_ex /s^-1"}, Axes → None,
 BaseStyle → {FontSize → 13}, Frame → True, PlotTheme → "Monochrome",
 PlotLegends → {"linear numeric", "linear first order", "linear second order"}]
w1x = 50; ran1 = 8000; ran2 = 8000; ran3 = 500;
Plot[{fourstarexact[x, -850, 2550, -4250, w1x, 140, 350,
   350, 700, 0.92, 0.05, 0.025, 0.005], fourstarfirstorder[x, -850,
   2550, -4250, w1x, 140, 350, 350, 700, 0.92, 0.05, 0.025, 0.005]},
 {x, -ran1, ran2}, PlotRange → {{-ran1, ran2}, {0, ran3}}, GridLines → None,
 FrameLabel → {"ΔΩ /s^-1", "R_ex /s^-1"}, Axes → None,
 BaseStyle → {FontSize → 13}, Frame → True, PlotTheme → "Monochrome",
 PlotLegends → {"star numeric", "linear first order"}]
Plot[{fourkiteexact[x, -850, 2550, -4250, w1x, 140, 350, 350, 700, 0.92,
   0.05, 0.025, 0.005], fourkitefirstorder[x, -850, 2550, -4250, w1x,
   140, 350, 350, 700, 0.92, 0.05, 0.025, 0.005], fourkitewoodbury[x,
   -850, 2550, -4250, w1x, 140, 350, 350, 700, 0.92, 0.05, 0.025, 0.005]},
 {x, -ran1, ran2}, PlotRange → {{-ran1, ran2}, {0, ran3}}, GridLines → None,
 FrameLabel → {"ΔΩ /s^-1", "R_ex /s^-1"}, Axes → None,
 BaseStyle → {FontSize → 13}, Frame → True, PlotTheme → "Monochrome",
 PlotLegends → {"kite numeric", "kite first order", "kite Woodbury"}]
```

```
Plot[{fourlinearexact[x, -850, 2550, -4250, w1x, 140, 350, 350, 700, 0.92,
    0.05, 0.025, 0.005], fourlinearfirstorder[x, -850, 2550, -4250, w1x,
    140, 350, 350, 700, 0.92, 0.05, 0.025, 0.005], fourlinearsecondorder[x,
    -850, 2550, -4250, w1x, 140, 350, 350, 700, 0.92, 0.05, 0.025, 0.005]},
 {x, -ran1, ran2}, PlotRange → {{-ran1, ran2}, {0, ran3}}, GridLines → None,
 FrameLabel → {"ΔΩ /s^-1", "R_ex /s^-1"}, Axes → None,
 BaseStyle → {FontSize → 13}, Frame → True, PlotTheme → "Monochrome",
 PlotLegends → {"linear numeric", "linear first order", "linear second order"}]
```

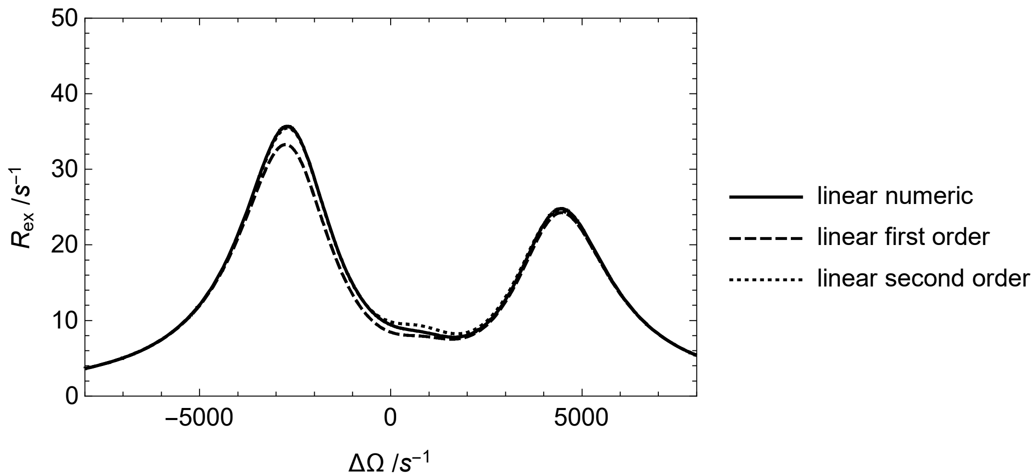
Out[1028]=



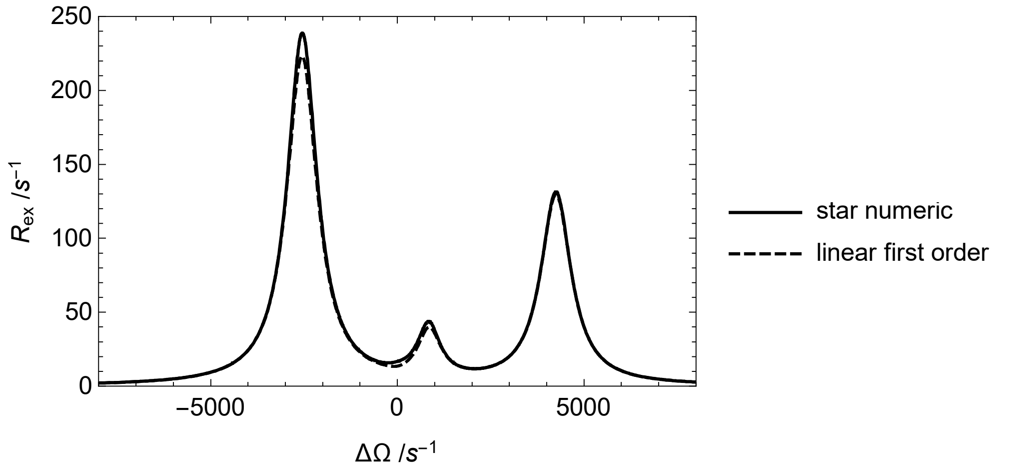
Out[1029]=



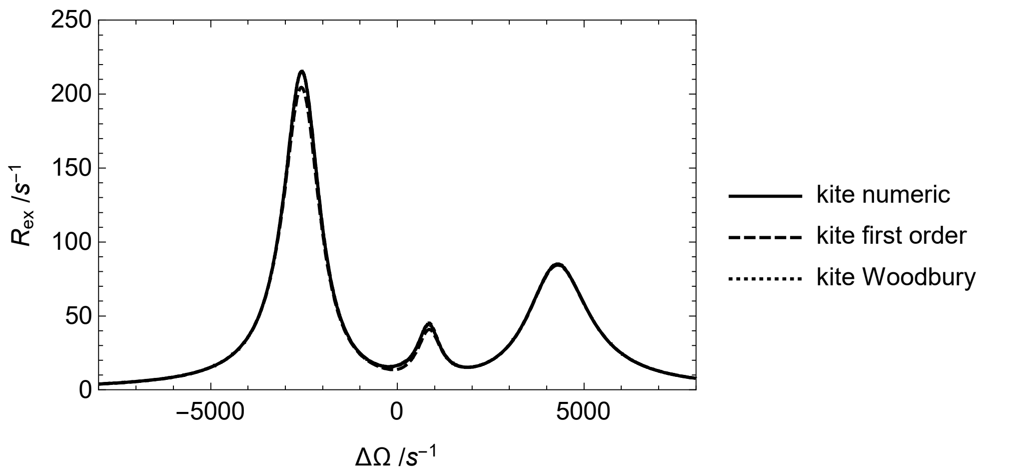
Out[1030]=



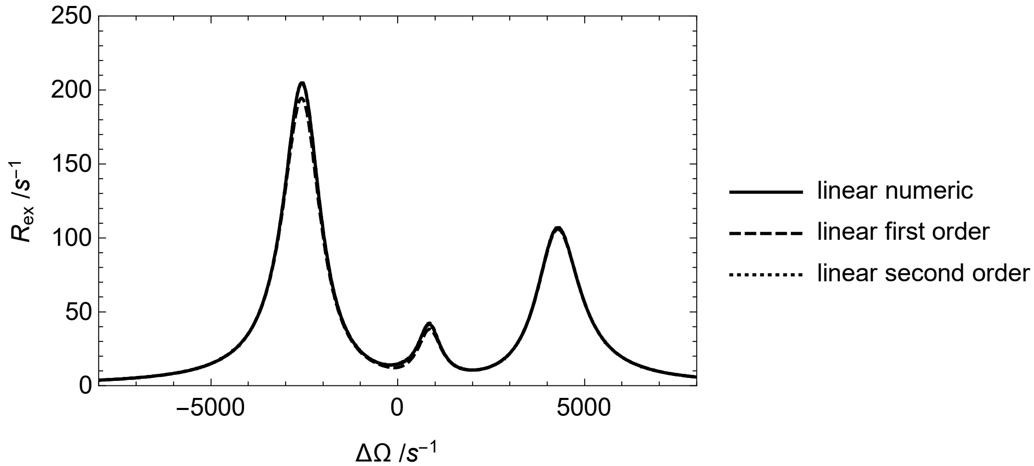
Out[1032]=



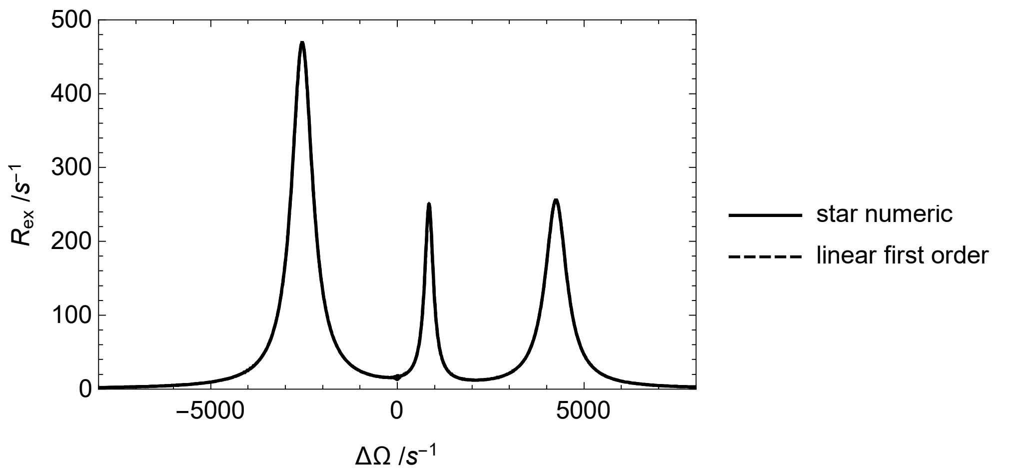
Out[1033]=



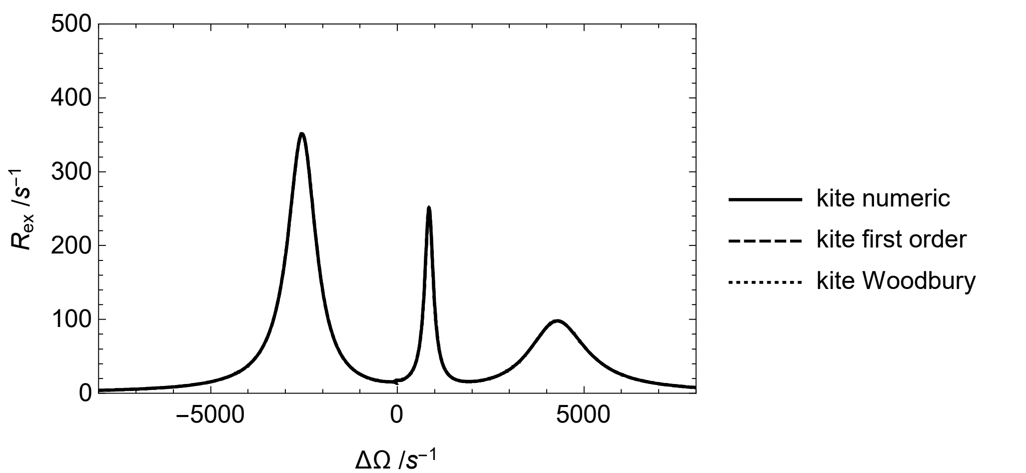
Out[1034]=



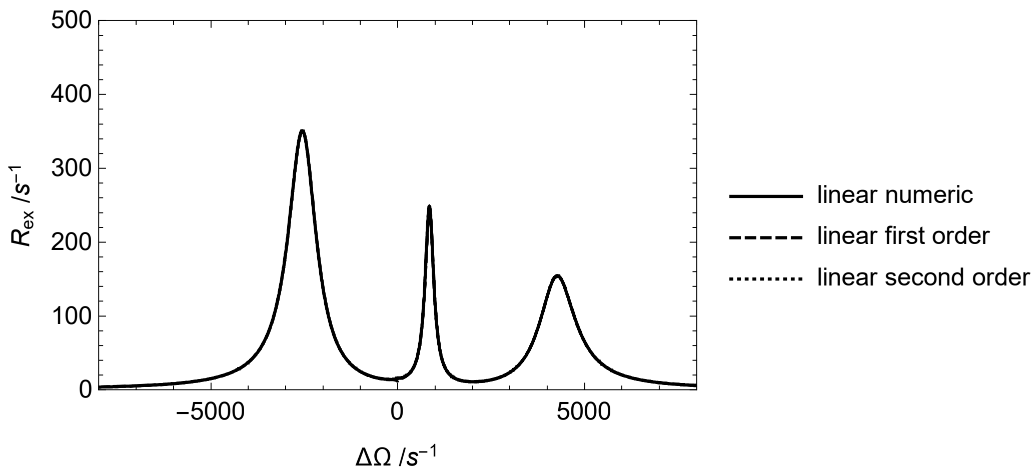
Out[1036]=



Out[1037]=



Out[1038]=

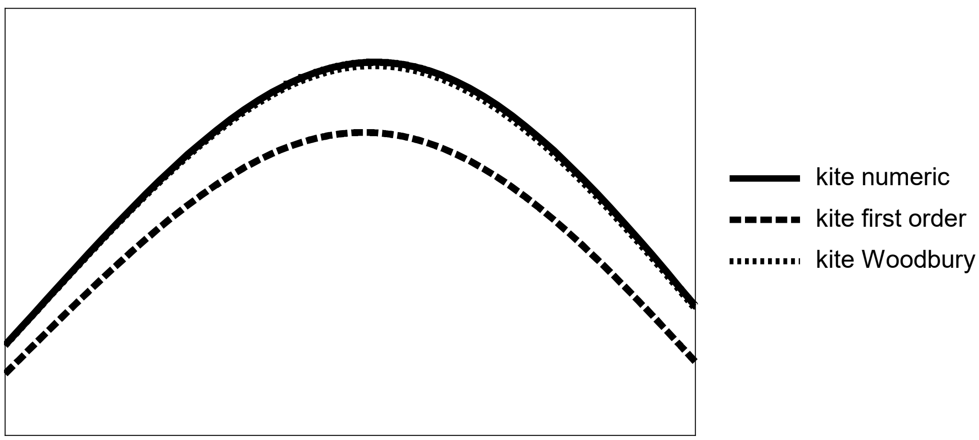


In[1039]:=

```
a = 0.85;
b = 0.7;
d = 3;
y = 500;
f = 500;
g = 1000;
h = 500;
f1 = -3000;
f2 = -2200;
f3 = 100;
f4 = 160;
o = 0.01;
Plot[{fourkiteexact[x, a * -1000, a * 3000,
    a * -5000, y, b * 200, b * h, b * f, b * g, 0.92, 0.05, 0.025, 0.005],
   fourkitefirstorder[x, a * -1000, a * 3000, a * -5000, y, b * 200, b * h, b * f,
    b * g, 0.92, 0.05, 0.025, 0.005], fourkitewoodbury[x, a * -1000, a * 3000,
    a * -5000, y, b * 200, b * h, b * f, b * g, 0.92, 0.05, 0.025, 0.005]},
 {x, f1, f2}, PlotRange → {{f1, f2}, {f3, f4}}, FrameLabel → None,
 GridLines → None, Axes → None, BaseStyle → {FontSize → 13},
 Frame → True, FrameTicks → None, PlotTheme → "Monochrome",
 PlotLegends → {"kite numeric", "kite first order", "kite Woodbury"},
 PlotStyle → {Thickness[o]}]
a = 0.85;
b = 0.7;
d = 3;
y = 1250;
f = 500;
g = 1000;
h = 500;
f1 = 0;
```

```
f2 = 2000;
f3 = 8;
f4 = 15;
Plot[{fourkiteexact[x, a * -1000, a * 3000,
    a * -5000, y, b * 200, b * h, b * f, b * g, 0.92, 0.05, 0.025, 0.005],
   fourkitefirstorder[x, a * -1000, a * 3000, a * -5000, y, b * 200, b * h, b * f,
    b * g, 0.92, 0.05, 0.025, 0.005], fourkitewoodbury[x, a * -1000, a * 3000,
    a * -5000, y, b * 200, b * h, b * f, b * g, 0.92, 0.05, 0.025, 0.005]},
 {x, f1, f2}, PlotRange → {{f1, f2}, {f3, f4}}, FrameTicks → None,
 GridLines → None, FrameLabel → None, Axes → None,
 BaseStyle → {FontSize → 13}, Frame → True, PlotTheme → "Monochrome",
 PlotLegends → {"kite numeric", "kite first order", "kite Woodbury"},
 PlotStyle → {Thickness[0.01]}]
```

Out[1040]=



Out[1042]=