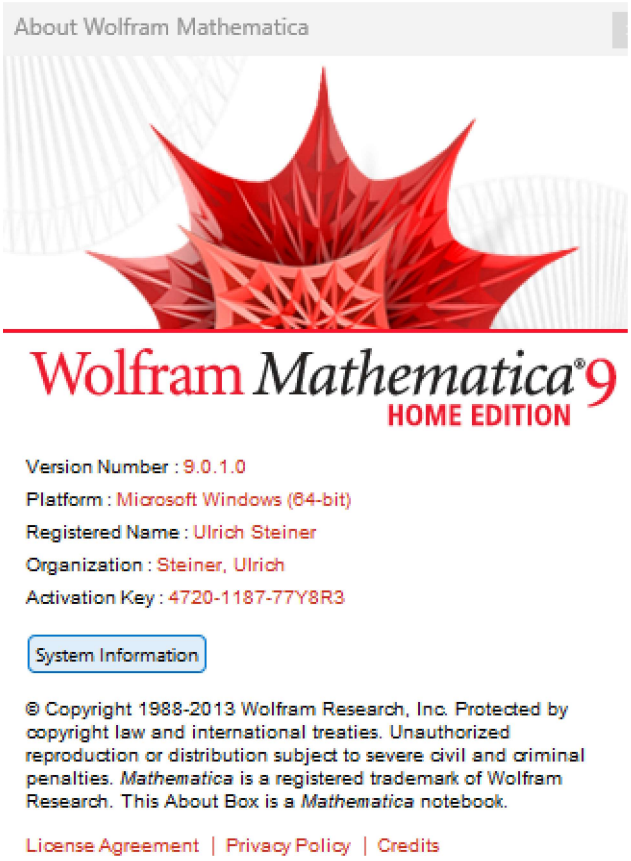


Mathematica Notebook for Calculating the Spin- and Reaction Dynamics of Rigidly Linked Radical Pairs

basic version developed by

Ulrich E. Steiner, University of Konstanz, Konstanz and
Nikita N. Lukzen, International Tomography Institute, Novosibirsk.

basic theory described in

Lukzen NN, Klein JH, Lambert C, Steiner UE. Z Physik Chem N F. 2017;231(2):197-223.

implementation of relaxation according to Nakashima-Zwanzig theory, following:

P. Fay, L. P. Lindoy and D. E. Manolopoulos, J. Chem. Phys., 2019, 151, 154117.

current version, extended for reversibly coupled RP to a precursor S1 state

by Ulrich E. Steiner

Definition of Operators

```
============================================================
============
```

```
U2 = {{1, 0}, {0, 1}};
U3 = {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}};
U8 = KroneckerProduct[U2, U2, U2];
U12 = KroneckerProduct[U2, U2, U3];
U15 = IdentityMatrix[15];
sx = 1 / 2 * {{0, 1}, {1, 0}};
sy = 1 / 2 * {{0, -I}, {I, 0}};
sz = 1 / 2 * {{1, 0}, {0, -1}};
Ix = 1 / Sqrt[2] * {{0, 1, 0}, {1, 0, 1}, {0, 1, 0}};
Iy = I / Sqrt[2] * {{0, -1, 0}, {1, 0, -1}, {0, 1, 0}};
Iz = {{1, 0, 0}, {0, 0, 0}, {0, 0, -1}};
S1x = KroneckerProduct[sx, U2, U3];
S1y = KroneckerProduct[sy, U2, U3];
S1z = KroneckerProduct[sz, U2, U3];
S2x = KroneckerProduct[U2, sx, U3];
S2y = KroneckerProduct[U2, sy, U3];
S2z = KroneckerProduct[U2, sz, U3];
INx = KroneckerProduct[U2, U2, Ix];
INy = KroneckerProduct[U2, U2, Iy];
INz = KroneckerProduct[U2, U2, Iz];
S1p = S1x + I * S1y;
S1m = S1x - I * S1y;
INp = INx + I * INy;
INm = INx - I * INy;
S1 = {S1x, S1y, S1z};
IN = {INx, INy, INz};
QS = 1 / 4 * U12 - S1x.S2x - S1y.S2y - S1z.S2z;
QT = U12 - QS;
ψTp = {1, 0, 0, 0};
ψTm = {0, 0, 0, 1};
ψT0 = {0, 1, 1, 0} / Sqrt[2];
ψS = {0, 1, -1, 0} / Sqrt[2];
ψSTpcoh = (ψS + ψTp) / Sqrt[2];
PSTpcoh = Outer[Times, ψSTpcoh, ψSTpcoh*];
QSTpcoh = KroneckerProduct[PSTpcoh, U3];
PT0 = Outer[Times, ψT0, ψT0*];
PTp = Outer[Times, ψTp, ψTp*];
PTm = Outer[Times, ψTm, ψTm*];
qS = Outer[Times, ψS, ψS*];
QT0 = KroneckerProduct[PT0, U3];
QTp = KroneckerProduct[PTp, U3];
QTm = KroneckerProduct[PTm, U3];
UN1 = {{1, 0, 0}, {0, 0, 0}, {0, 0, 0}};
UN0 = {{0, 0, 0}, {0, 1, 0}, {0, 0, 0}};
UNm1 = {{0, 0, 0}, {0, 0, 0}, {0, 0, 1}};
QTpm = QT - QT0;
de[i_, j_] := If[i == j, 1.0, 0];
```

```
(*Operators in {15,15}*)
QS1 = ConstantArray[0, {15, 15}];
QS1[[13, 13]] = 1; QS1[[14, 14]] = 1; QS1[[15, 15]] = 1;
QS1sup = KroneckerProduct[QS1, QS1^T];
QS15 = ArrayPad[QS, {{0, 3}, {0, 3}}, 0];
QT15 = ArrayPad[QT, {{0, 3}, {0, 3}}, 0];
U1512 = IdentityMatrix[15] - QS1;
Pex = {{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, 0}, {0, 0, 0}, {0, 0, 0}, {1, 0, 0}, {0, 1, 0}, {0, 0, 1}};
Pin = {{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}, {0, 0, 0},
    {0, 0, 0}, {0, 0, 0}, {0, 0, 0}, {0, 0, 0}, {0, 0, 0}};
Qex = {{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}, {0, 0, 0},
    {0, 0, 0}, {0, 0, 0}, {0, 0, 0}, {0, 0, 0}, {0, 0, 0}};
Qin = {{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, 0},
    {0, 0, 0}, {0, 0, 0}, {1, 0, 0}, {0, 1, 0}, {0, 0, 1}};
linNr144[a_, b_, c_, d_] := d + 3 * (c - 1) + 3 * 4 * (b - 1) + 3 * 4 * 3 * (a - 1)
linNr225[a_, b_, c_, d_] := d + 3 * (c - 1) + 5 * 3 * (b - 1) + 3 * 5 * 3 * (a - 1)
LsupRM4 = ConstantArray[0, {4, 3, 4, 3, 4, 3, 4, 3}];
LsupRM5 = ConstantArray[0, {5, 3, 4, 3, 5, 3, 4, 3}];
LsupR225 = ConstantArray[0, {225, 225}];

(*==========  Verschwinden von S1 durch CS*)
QSsup = KroneckerProduct[QS15, QS15^T];
(*========== S1 Rückbildung aus 1CSS*)
S1ausrCS =
  KroneckerProduct[T15.Qin.Qex^T.T15m, (T15.Qex.Qin^T.T15m)^T];
(*==========  Bildung von 1CSS durch CS aus S1*)
SCSSausCS =
  KroneckerProduct[T15.Pin.Pex^T, (Pex.Pin^T.T15m)^T];

(*SCSSperkrCR=KroneckerProduct[QS15,QS15^T];*)
SCSSperkrCR = 1 / 2
   (KroneckerProduct[QS15, U15] + KroneckerProduct[U15, QS15^T]);

(*jetzt mit Haberkornversion
    von Abreaktion per krCS nach S1
   ursprünglich:
    SCSSperkrCR=KroneckerProduct[QS15,QS15^T];
 =========
 Verschwinden von 1CSS durch Rückbildung von S1*)
sq2 = 1 / Sqrt[2];
T15m = {{1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0},
    {0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 1, 0, 0, 0, 0, 0,
     0, 0, 0, 0, 0, 0, 0}, sq2 {0, 0, 0, 1, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0},
    sq2 {0, 0, 0, 0, 1, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0},
    sq2 {0, 0, 0, 0, 0, 1, 0, 0, 1, 0, 0, 0, 0, 0, 0},
```

```
    sq2 {0, 0, 0, -1, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0},
    sq2 {0, 0, 0, 0, -1, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0},
    sq2 {0, 0, 0, 0, 0, -1, 0, 0, 1, 0, 0, 0, 0, 0, 0},
    {0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0,
     0, 0, 1, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0},
    {0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0,
     0, 0, 0, 0, 0, 1, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1}};
T15 = Inverse[T15m];
```

==========

==========

Parameters

```
ΔA = 15;
DAR = (ΔA * ΔA) * 0.0176^2;
GG1 = gddg = 0;(*g-tensor anisotropie of radical 1*)
GG2 = 0;(*g-tensor anisotropie of radical 2*)
a = 10 * 0.0176;
J = 5 * 0.176;
kdeph = 0.1;
Tlong = Infinity;(*wenn ks = 0.00125 Tlong = inf völlig äquivalent!*)
τ = 0.6;
(*hier folgt alternativ die äquivalente Rechnung mit DARJ*)
DARJ = 0 * 5.0;
τJ = 0.055;
4 * DARJ * τJ;
ks = 0.001;
kt = 0.02;
kf = 0.25;
kCS = 1.0;
krCS = 0.025;
```

```
SETS1 = {{"kCS", "krCS", "kf", "ks", "kt", "kdeph",
    "Tlong", "τ", "2J/0.176", "ΔA, G", "DAR", "a,G"},
   {kCS, krCS, kf, ks, kt, kdeph, Tlong, τ, 2 J / 0.176, ΔA, DAR, a / 0.0176}};
SETS1 // TableForm
```

kCS	krCS	kf	ks	kt	kdeph	Tlong	τ	2J/0.176	ΔA, G
1.	0.025	0.25	0.001	0.02	0.1	∞	0.6	10.	15

```
kf * krCS / (kf + kCS)
```

```
0.005
```

Magnetic Field Values in mT

```
FeldSel = {0, 2, 5, 7, 9, 10, 11, 12, 13, 15, 17, 20, 25, 30, 40, 50, 60, 80, 100, 200};
nFull = nSel = Dimensions[FeldSel][[1]]
```

```
20
```

Parameters to be varied during run

```
ksA = {0.001};
ktA = {0.02};
kdephA = {0.1};
TlongA = {Infinity};
ΔAA = {15};
τA = {0.6};
aA = {1.} * 0.176;

PTab = Flatten[Table[{ks, kt, kdeph, Tlong, ΔA, τ, a}, {ks, ksA}, {kt, ktA},
    {kdeph, kdephA}, {Tlong, TlongA}, {ΔA, ΔAA}, {τ, τA}, {a, aA}], 6]
Np = Dimensions[PTab][[1]]
```

```
{{0.001, 0.02, 0.1, ∞, 15, 0.6, 0.176}}
```

```
1
```

```
SETS1 =
  {{"kCS", "krCS", "kf", "ks", "kt", "k_STD", "Tlong", "τ", "2J,G", "ΔA,G", "a,G"},
   {kCS, krCS, kf, ksA, ktA, kdephA, TlongA, τA, 2 J / 0.176, ΔAA, aA / 0.0176}};

SETS1 // TableForm
```

kCS	krCS	kf	ks	kt	k_{STD}	Tlong	τ	2J,G	ΔA,G	a,G
1.	0.025	0.25	0.001	0.02	0.1	∞	0.6	10.	15	10.

Observables of pure CSS dynamics

```
RPvsB = ConstantArray[0, {Np, nSel, 1000}];
(*total RP population in calculation without reversible S1 formation*)
TRPvsB = ConstantArray[0, {Np, nSel, 1000}];(*triplet part of
 RP population in calculation without reversible S1 formation*)
SRPvsB = ConstantArray[0, {Np, nSel, 1000}];
(*singlet part of RP population in
 calculation without reversible S1 formation*)
```

Observables of S1-coupled CSS dynamics

```
RPvsB225 = ConstantArray[0, {Np, nSel, 1000}];
(*total population (S1+RP) in calculation with reversible S1 formation*)
SRPvsB225 = ConstantArray[0, {Np, nSel, 1000}];
(*singlet RP population in calculation with reversible S1 formation*)
TRPvsB225 = ConstantArray[0, {Np, nSel, 1000}];
(*triplet RP population in calculation with reversible S1 formation*)
RPvsB225CSS = ConstantArray[0, {Np, nSel, 1000}];
(*total RP population in calculation with reversible S1 formation*)
S1pop225 = ConstantArray[0, {Np, nSel, 1000}];
(*(100x) S1-population in calculation with reversible S1 formation*)
```

```
Np = Dimensions[PTab][[1]]
PTab // TableForm
```

```
1
```

```
0.001    0.02    0.1    ∞    15    0.6    0.176
```

Quantum Dynamics Calculation

```
time0 = TimeUsed[];
Do[
 Do[
  (
   ω0 = FeldSel[[n]] * 0.176; (*FeldM0[[n]]*0.176  B0[[n]]*10*0.0176*)
   {ks, kt, kdeph, Tlong, ΔA, τ, a} = PTab[[np]];
   DAR = (ΔA * ΔA) * 0.0176^2;
H = a * (INx.S1x + INy.S1y + INz.S1z) +
      ω0 (S1z + S2z) - 2 J (S1x.S2x + S1y.S2y + S1z.S2z);
Ω = H - 1 / 2 I * (ks * QS + kt * QT);
   UT = Eigensystem[Ω];
   UTH = Eigensystem[H];
U = UT[[2]]^T;
   UH = UTH[[2]]^T;
   ω = DiagonalMatrix[UT[[1]]];
   ωH = DiagonalMatrix[UTH[[1]]];
   S1ω = ArrayPad[ω, 3, 0];
   S1ωH = ArrayPad[ω, 3, 0];
(*Superoperators*)
   Usup = KroneckerProduct[U, U*];
Usupm1 = Inverse[Usup];
λsup = -KroneckerProduct[ω, U12] + KroneckerProduct[U12, ω*];
   Hsup = KroneckerProduct[H, U12] - KroneckerProduct[U12, H^T];
   Ksup = 1 / 2 * ks * (KroneckerProduct[QS, U12] + KroneckerProduct[U12, QS^T]) +
     1 / 2 * kt * (KroneckerProduct[QT, U12] + KroneckerProduct[U12, QT^T]);

   (*Relaxation*)
   Jsup = DiagonalMatrix[τ / (1 - I * τ * Diagonal[λsup])];
   Ha1 = S1z.INz - 0.25 * (S1p.INm + S1m.INp);
   Ha21 = S1p.INz + S1z.INp;
   Ha22 = S1m.INz + S1z.INm;
   Ha31 = S1p.INp;
   Ha32 = S1m.INm;
Ha1sup = KroneckerProduct[Ha1, U12] - KroneckerProduct[U12, Ha1^T];
   Ha21sup = KroneckerProduct[Ha21, U12] - KroneckerProduct[U12, Ha21^T];
   Ha22sup = KroneckerProduct[Ha22, U12] - KroneckerProduct[U12, Ha22^T];
   Ha31sup = KroneckerProduct[Ha31, U12] - KroneckerProduct[U12, Ha31^T];
   Ha32sup = KroneckerProduct[Ha32, U12] - KroneckerProduct[U12, Ha32^T];
RNZ11 = -4 / 45 * DAR * Ha1sup^T*.Usup.Jsup.Usupm1.Ha1sup // Simplify;
RNZ21 = -1 / 30 * DAR * Ha21sup^T*.Usup.Jsup.Usupm1.Ha21sup // Simplify;
RNZ22 = -1 / 30 * DAR * Ha22sup^T*.Usup.Jsup.Usupm1.Ha22sup // Simplify;
```

```
RNZ31 = -1 / 30 * DAR * Ha31sup^T*.Usup.Jsup.Usupm1.Ha31sup // Simplify;
RNZ32 = -1 / 30 * DAR * Ha32sup^T*.Usup.Jsup.Usupm1.Ha32sup // Simplify;
RNZ = RNZ11 + RNZ21 + RNZ22 + RNZ31 + RNZ32;

HaJ = (U12 / 2 + 2 * (S1x.S2x + S1y.S2y + S1z.S2z));
HaJsup = KroneckerProduct[HaJ, U12] - KroneckerProduct[U12, HaJ^T];
    JsupJ = DiagonalMatrix[τJ / (1 - I * τJ * Diagonal[λsup])];
    RNZJ = -DARJ * HaJsup^T*.Usup.JsupJ.Usupm1.HaJsup // Simplify;
```

(*dephasing |||||||||||||||||||||*)

```
de[i_, j_] := If[i == j, 1.0, 0];
    s2 = 1 / Sqrt[2];
Tk = {{0, s2, -s2, 0}, {0, s2, s2, 0}, {1, 0, 0, 0}, {0, 0, 0, 1}};
T1k = {{0, 0, 1, 0}, {s2, s2, 0, 0}, {-s2, s2, 0, 0}, {0, 0, 0, 1}};
TEk = Inverse[Tk];
    TE1k = Inverse[T1k];
Qk = ConstantArray[0, {16, 16}];
    Gk = ConstantArray[0, {16, 16}];
Do[
     Do[
      Do[
       Do[
        (Ik = mk + 4 * (lk - 1);
         Kk = kk + 4 * (ik - 1);
         Qk[[Ik, Kk]] = Tk[[ik, lk]] * TEk[[mk, kk]];
         Gk[[Ik, Kk]] = T1k[[ik, lk]] * TE1k[[mk, kk]];),
        {mk, 4}],
       {kk, 4}],
      {lk, 4}],
     {ik, 4}];
REL = ConstantArray[0, {16, 16}];
REL[[2, 2]] = -kdeph; (*ST_0 - ST_0 dephasing*)
REL[[3, 3]] = -kdeph; (* ST_+ - ST_+ dephasing*)
REL[[4, 4]] = -kdeph;  (*etc,
    order is: 1 - SS, 2 - ST_0, 3- ST_+, 4 - ST_-, 5 - T_0S, 6- T_0T_0, etc *)
REL[[5, 5]] = -kdeph;
REL[[9, 9]] = -kdeph;
REL[[13, 13]] = -kdeph;
RELDH = Qk.REL.Gk;
ZeemRephase = ConstantArray[0, {144, 144}];
Do[
     Do[
      Do[
       Do[
        Do[
         Do[
          Do[
           Do[
            (II = BB + (bb - 1) * 3 + 12 * (AA + 3 * (aa - 1) - 1);
             JJ = DD + (dd - 1) * 3 + 12 * (CC + 3 * (cc - 1) - 1);
             ZeemRephase[[II, JJ]] =
              RELDH[[bb + 4 * (aa - 1), dd + 4 * (cc - 1)]] * de[AA, CC] * de[BB, DD];),
```

```
          {DD, 3}],
         {dd, 4}],
        {CC, 3}],
       {cc, 4}],
      {BB, 3}],
     {bb, 4}],
    {AA, 3}],
   {aa, 4}];
  (*||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||
  *)
(*Tlong*)
  RelaT1 = ConstantArray[0, {4, 4}];
  RelaT1[[1, 1]] = -1 / 2 / Tlong;
RelaT1[[1, 4]] = 1 / 2 / Tlong;
RelaT1[[2, 2]] = -1 / Tlong;
RelaT1[[3, 3]] = -1 / Tlong;
RelaT1[[4, 1]] = 1 / 2 / Tlong;
RelaT1[[4, 4]] = -1 / 2 / Tlong;
  ZeemRelaxT1 = ConstantArray[0, {144, 144}];

  Do[
   Do[
    Do[
     Do[
      Do[
       Do[
        Do[
         Do[
          Do[(
            II = B1 + 6 * (b1 - 1) + 12 * (A1 + 6 * (a1 - 1) - 1);
            JJ = D1 + 6 * (d1 - 1) + 12 * (C1 + 6 * (c1 - 1) - 1);
            ZeemRelaxT1[[II, JJ]] =
             de[A1, C1] * de[B1, D1] * RelaT1[[b1 + 2 * (a1 - 1), d1 + 2 * (c1 - 1)]];
           ),
          {a1, 2}],
         {A1, 6}],
        {b1, 2}],
       {B1, 6}],
      {c1, 2}],
     {C1, 6}],
    {d1, 2}],
   {D1, 6}];
(*Rgta*)
B00 = ω0;
S1xsup = KroneckerProduct[S1x, U12] - KroneckerProduct[U12, S1x^T];
S1ysup = KroneckerProduct[S1y, U12] - KroneckerProduct[U12, S1y^T];
S1zsup = KroneckerProduct[S1z, U12] - KroneckerProduct[U12, S1z^T];

  S2xsup = KroneckerProduct[S2x, U12] - KroneckerProduct[U12, S2x^T];
S2ysup = KroneckerProduct[S2y, U12] - KroneckerProduct[U12, S2y^T];
S2zsup = KroneckerProduct[S2z, U12] - KroneckerProduct[U12, S2z^T];
```

```
JG = Jsup;
R1x = -B00 * B00 * GG1 * S1xsup^T* .Usup.JG.Usupm1.S1xsup / 40;
   R1y = -B00 * B00 *
     GG1 * S1ysup^T* .Usup.JG.Usupm1.S1ysup / 40;
R1z = -2.0 * B00 * B00 * GG1 * S1zsup^T* .Usup.JG.Usupm1.S1zsup / 60.0;

R2x = -B00 * B00 * GG2 * S2xsup^T* .Usup.JG.Usupm1.S2xsup / 40;
R2y = -B00 * B00 * GG2 * S2ysup^T* .Usup.JG.Usupm1.S2ysup / 40;
R2z = -2.0 * B00 * B00 * GG2 * S2zsup^T* .Usup.JG.Usupm1.S2zsup / 60.0;

Rgta = R1x + R1y + R1z + R2x + R2y + R2z;

LsupR = (-I * Hsup - Ksup + RNZ +
       RNZJ + ZeemRephase + ZeemRelaxT1 + Rgta) // Chop;


   (*Ergebnisse für rein innere CSS Kinetik *)
   dt = 1;
Prop = MatrixExp[LsupR * dt];
   RF = Flatten[QS / Tr[QS]];
   (*RF=Flatten[U12/12];*)

   time0 = TimeUsed[];
(*bei den folgenden Zeilen wurde darauf geachtet,
   dass jeder Befehl in einer eigenen Zeile steht:*)
   Do[RPvsB[[np, n, i]] = {(i - 1) * dt, Tr[ArrayReshape[RF, {12, 12}]] // Chop};
    SRPvsB[[np, n, i]] = {(i - 1) * dt, Tr[QS.ArrayReshape[RF, {12, 12}]] // Chop};
    RF = Prop.RF, {i, 1000}];
   timea = TimeUsed[];

(*New addition to
   include reversible S1 coupling*)
   Kontrolle = Table[LsupRM4[[a, b, c, d, as, bs, cs, ds]] =
      LsupR[[linNr144[a, b, c, d], linNr144[as, bs, cs, ds]]], {d,
      3}, {c, 4}, {b, 3}, {a, 4}, {ds, 3}, {cs, 4}, {bs, 3}, {as, 4}];
Do[LsupRM5[[a, b, c, d, as, bs, cs, ds]] =
      LsupRM4[[a, b, c, d, as, bs, cs, ds]], {d, 3}, {c, 4},
     {b, 3}, {a, 4}, {ds, 3}, {cs, 4}, {bs, 3}, {as, 4}]
Do[LsupR225[[linNr225[a, b, c, d], linNr225[as, bs, cs, ds]]] =
      LsupRM5[[a, b, c, d , as, bs, cs, ds]], {as, 5},
     {bs, 3}, {cs, 4}, {ds, 3}, {a, 5}, {b, 3}, {c, 4}, {d, 3}]
LsupR225kfkCSkrCS = LsupR225 - (kf + kCS) * QS1sup +
      krCS * S1ausrCS + kCS * SCSSausCS - krCS * SCSSperkrCR;

dt = 1;
Prop225kfkCSkrCS = MatrixExp[LsupR225kfkCSkrCS * dt];
RFS1 = Flatten[QS1 / Tr[QS1]];

timeb0 = TimeUsed[];
   Do[X = ArrayReshape[RFS1, {15, 15}] // Chop;
    SRPvsB225[[np, n, i]] = {(i - 1) * dt, Tr[QS15.X]};
```

```
    RPvsB225[[np, n, i]] = {(i - 1) * dt, Tr[U1512.X]};
    S1pop225[[np, n, i]] = {(i - 1) * dt, 100 * Tr[QS1.X]};
    RFS1 = Prop225kfkCSkrCS.RFS1;, {i, 1000}];
   If[n == 1, WriteString[$Output, "\n", n, " ", np, "    "],
    WriteString[$Output, n, " ", np, "    "]];
   timeb = TimeUsed[]
  ),
  {n, nSel}];
 x = 1.23,
 {np, Np}]
time1 = TimeUsed[];
Dauera = timea - time0
Dauerb = timeb - timeb0
Dauer = time1 - time0
```

```
1 1    2 1    3 1    4 1    5 1    6 1    7 1    8 1    9 1    10 1    11 1    12 1    13 1    14
0.078

0.093

0.578
```

```
SRPvsB[[1, 1, 1 ;; 10]]
```

```
{{0, 1}, {1, 0.983246}, {2, 0.971729}, {3, 0.975986}, {4, 0.968114},
 {5, 0.954095}, {6, 0.952964}, {7, 0.950201}, {8, 0.938181}, {9, 0.932325}}
```

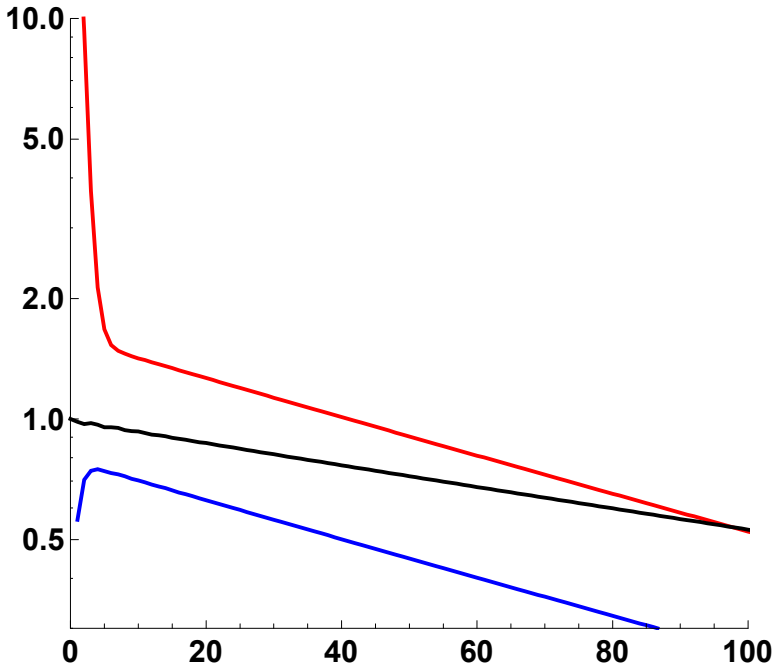
```
Dimensions[SRPvsB]
```

```
{1, 20, 1000, 2}
```

```
DCyan = RGBColor[0, 0.2, 0.2]
```

```
RGBColor[0, 0.2, 0.2]
```

```
ListLogPlot[{SRPvsB225[[1, 1]], S1pop225[[1, 1]], SRPvsB[[1, 1]]}, PlotStyle →
  {{Thick, Blue}, {Thick, Red}, {Thick, Black}, {Thick, Orange}, {Thick, Cyan}},
 BaseStyle -> {FontFamily → "Arial", FontWeight → "Bold", FontSize → 16},
 PlotRange → {{0.0, 100}, {0.3, 10}},
 Joined → True, ImageSize → 400, AspectRatio → 0.9]
```



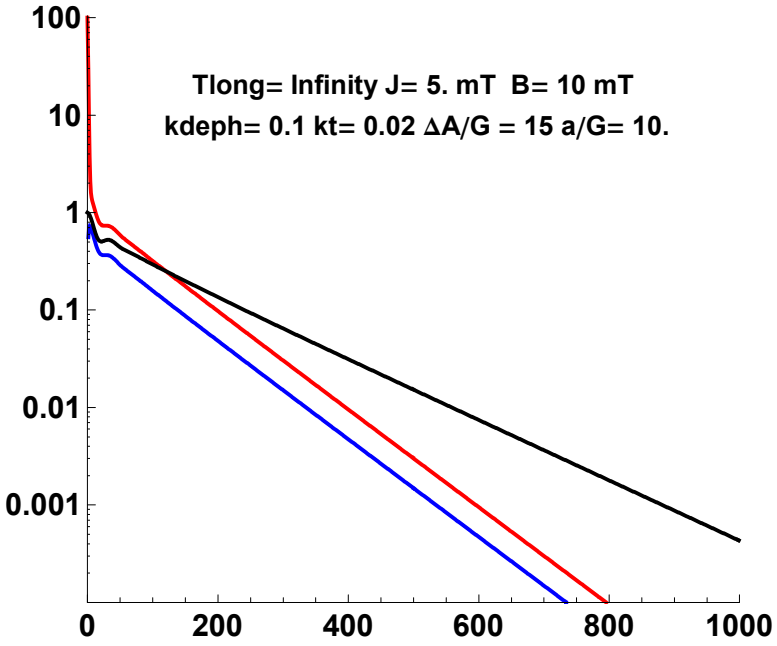

```
FeldSel
```

```
{0, 2, 5, 7, 9, 10, 11, 12, 13, 15, 17, 20, 25, 30, 40, 50, 60, 80, 100, 200}
```

```
FeldSel[[9]]
```

```
13
```

```
n = 6;
ListLogPlot[{SRPvsB225[[1, n]], S1pop225[[1, n]], SRPvsB[[1, n]]}, PlotStyle →
  {{Thick, Blue}, {Thick, Red}, {Thick, Black}, {Thick, Orange}, {Thick, Cyan}},
 BaseStyle -> {FontFamily → "Arial", FontWeight → "Bold", FontSize → 16},
 PlotRange → {{0.0, 1000}, {0.0001, 105}},
 Joined → True, ImageSize → 400, AspectRatio → 0.9,
 Epilog → Inset[Style[StringJoin["Tlong= ", ToString[Tlong], " ", "J= ",
     ToString[J / 0.176], " mT", "  B= ", ToString[FeldSel[[n]]], " mT",
     "\n", " kdeph= ", ToString[kdeph], " kt= ", ToString[kt], " ΔA/G = ",
     ToString[ΔA], " a/G= ", ToString[a / 0.0176]], Bold, 14], {500, 2.5}]]
```



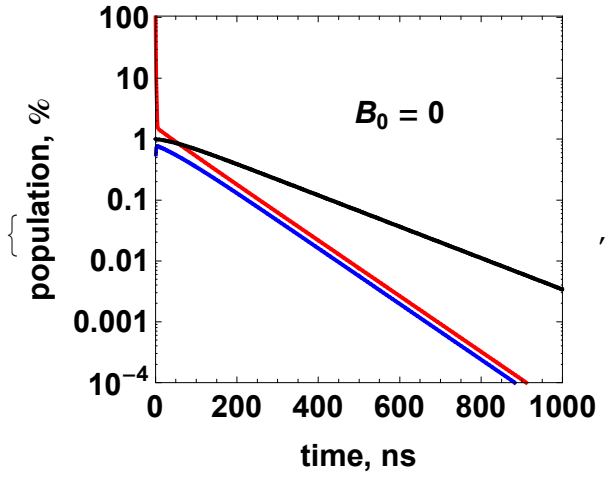

```
Epilog → Inset[
  Style[StringJoin["Tlong= ", ToString[Tlong], " ", "J= ", ToString[J / 0.176],
    " mT", "  B= ", ToString[FeldSel[[n]]], " mT", "\n", " kdeph= ",
    ToString[kdeph], " kt= ", ToString[kt], " ΔA= ", ToString[ΔA],
    " a/G= ", ToString[a / 0.0176]], Bold, 14], {500, 2.5}]
```

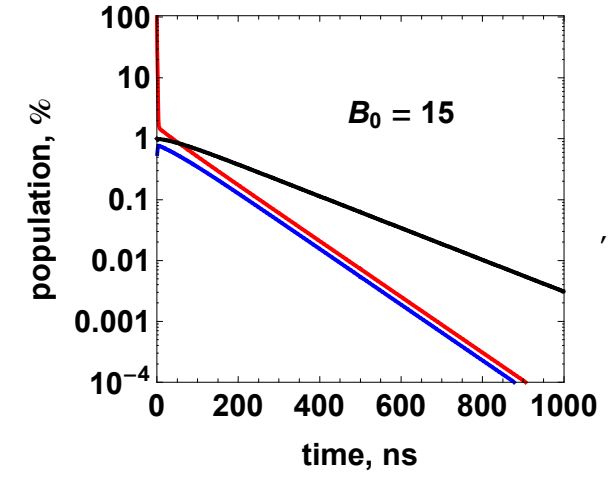
```
Epilog → Inset[Tlong= Infinity J= 5. mT  B= 10 mT
 kdeph= 0.1 kt= 0.02 ΔA= 15 a/G= 10., {500, 2.5}]
```

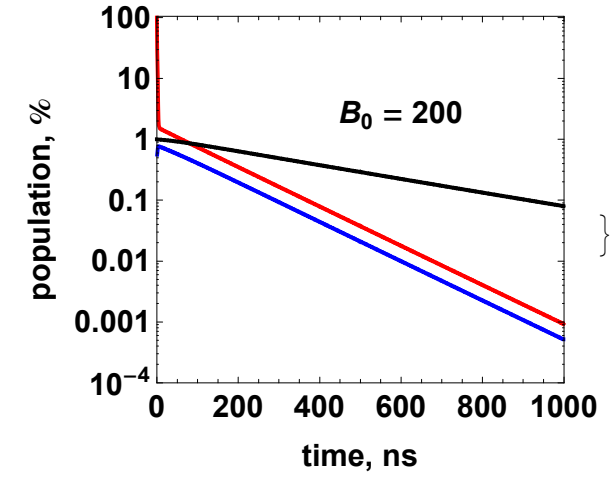
```
SETS1 // TableForm
Xa0 = Table[ListLogPlot[{RPvsB225[[1, n]], S1pop225[[1, n]], RPvsB[[1, n]]},
    PlotStyle → {{Thick, Blue}, {Thick, Red},
      {Thick, Black}, {Thick, Orange}, {Thick, Cyan}},
    BaseStyle -> {FontFamily → "Arial", FontWeight → "Bold", FontSize → 16},
    PlotRange → {{0.0, 1000}, {0.0001, 105}},
    Joined → True, ImageSize → 300, AspectRatio → 0.9,
    Epilog → Inset[StringJoin["B0 = ", ToString[FeldSel[[n]]]], {600, 1}],
    Frame → True, FrameLabel → {"time, ns", "population, %"}], {n, nSel}];
```

kCS	krCS	kf	ks	kt	k_{STD}	Tlong	τ	2J,G	ΔA,G	a,G
1.	0.025	0.25	0.001	0.02	0.1	∞	0.6	10.	15	10.

```
Xa0[[{1, 10, 20}]]
```


100
10
1
0.1
0.01
0.001
10^{-4}
population, %
B_0 = 0
0
200
400
600
800
1000
time, ns


100
10
1
0.1
0.01
0.001
10^{-4}
population, %
B_0 = 15
0
200
400
600
800
1000
time, ns


100
10
1
0.1
0.01
0.001
10^{-4}
population, %
B_0 = 200
0
200
400
600
800
1000
time, ns

Determination of exponential rate constants

==========

RPvsB225

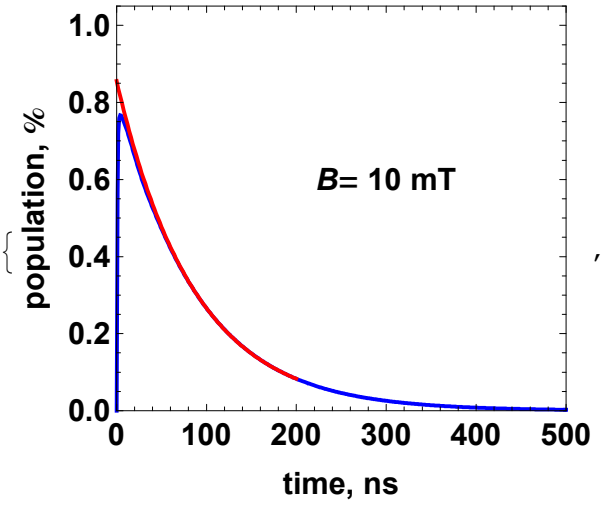
```
Lsl[x_, xa_, xb_] := Log[x[[xa, 2]] / x[[xb, 2]]] / (x[[xb, 1]] - x[[xa, 1]])
LA[x_, xa_, xb_] := Exp[Log[x[[xa, 2]]] + Lsl[x, xa, xb] * x[[xa, 1]]]
kCSS = ConstantArray[0, {Np, nSel, 2}];
ACSS = ConstantArray[0, {Np, nSel, 2}];
Do[(
  m = Lsl[RPvsB225[[np, n]], 200, 400] // Chop;
  Amp = LA[RPvsB225[[np, n]], 200, 400] // Chop;
  ACSS[[np, n]] = {FeldSel[[n]], Amp};
  kCSS[[np, n]] = {FeldSel[[n]], 10^9 m}),
 {np, Np}, {n, nSel}]
```

```
kCSS
```

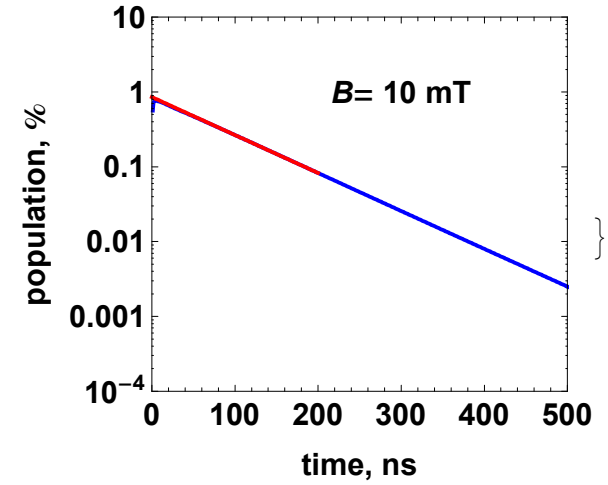
$$\{\{\{0, 1.04243\times10^{7}\}, \{2, 1.05383\times10^{7}\}, \{5, 1.09804\times10^{7}\}, \{7, 1.14919\times10^{7}\},$$
$$\{9, 1.1724\times10^{7}\}, \{10, 1.16817\times10^{7}\}, \{11, 1.16346\times10^{7}\}, \{12, 1.15266\times10^{7}\},$$
$$\{13, 1.12502\times10^{7}\}, \{15, 1.04755\times10^{7}\}, \{17, 9.85549\times10^{6}\}, \{20, 9.21646\times10^{6}\},$$
$$\{25, 8.57113\times10^{6}\}, \{30, 8.2066\times10^{6}\}, \{40, 7.84896\times10^{6}\}, \{50, 7.69023\times10^{6}\},$$
$$\{60, 7.60692\times10^{6}\}, \{80, 7.52656\times10^{6}\}, \{100, 7.49031\times10^{6}\}, \{200, 7.44296\times10^{6}\}\}\}$$

```
RPsim = CSSsim = Table[{t, ACSS[[np, n, 2]] * Exp[-kCSS[[np, n, 2]] / 10^9 * t]},
     {np, Np}, {n, nSel}, {t, 0, 200, 2}];
```

```
n = 6; np = 1;
{ListPlot[{RPvsB225[[np, n]], RPsim[[np, n]]},
  PlotStyle → {{Thick, Blue}, {Thick, Red}, {Thick, Black},
    {Thick, DCyan, Dashed}, {Thick, Black, Dashed}, {Thick, DCyan, Dashed}},
  PlotRange → {{0.0, 500}, {0.0, 1.05}}, Joined → True,
  BaseStyle -> {FontFamily → "Arial", FontWeight → "Bold", FontSize → 16},
  AspectRatio → 0.9, ImageSize → 300, Frame → True,
  FrameLabel → {"time, ns", "population, %"},
  Epilog → Inset[StringJoin["B= ", ToString[FeldSel[[n]]], " mT"], {300, 0.6}]],
 ListLogPlot[{RPvsB225[[np, n]], RPsim[[np, n]]},
  PlotStyle → {{Thick, Blue}, {Thick, Red}, {Thick, Black},
    {Thick, DCyan, Dashed}, {Thick, Black, Dashed}, {Thick, DCyan, Dashed}},
  PlotRange → {{0.0, 500}, {0.0001, 10}}, Joined → True,
  BaseStyle -> {FontFamily → "Arial", FontWeight → "Bold", FontSize → 16},
  AspectRatio → 0.9, ImageSize → 300, Frame → True,
  FrameLabel → {"time, ns", "population, %"}, Epilog →
   Inset[StringJoin["B= ", ToString[FeldSel[[n]]], " mT"], {300, Log[1]}]]}
```



,



}

```
FeldSel
```

```
{0, 2, 5, 7, 9, 10, 11, 12, 13, 15, 17, 20, 25, 30, 40, 50, 60, 80, 100, 200}
```

==========

==========

S1pop225

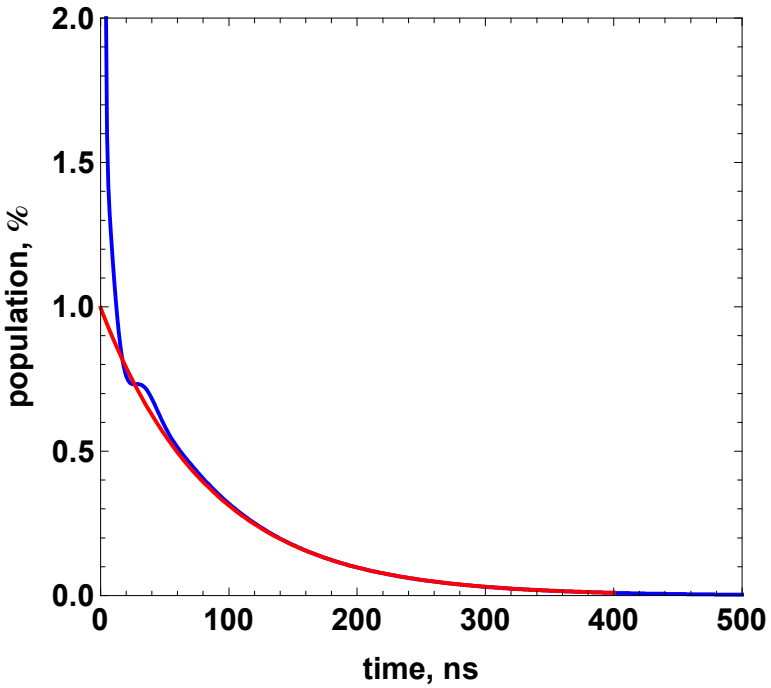
```
Lsl[x_, xa_, xb_] := Log[x[[xa, 2]] / x[[xb, 2]]] / (x[[xb, 1]] - x[[xa, 1]])
LA[x_, xa_, xb_] := Exp[Log[x[[xa, 2]]] + Lsl[x, xa, xb] * x[[xa, 1]]]
kslowMq = ConstantArray[0, {Np, nSel, 2}];
AslowMq = ConstantArray[0, {Np, nSel, 2}];
Do[(
  m = Lsl[S1pop225[[np, n]], 200, 400] // Chop;
  Amp = LA[S1pop225[[np, n]], 200, 400] // Chop;
  AslowMq[[np, n]] = {FeldSel[[n]], Amp};
  kslowMq[[np, n]] = {FeldSel[[n]], 10^9 m}),
 {np, Np}, {n, nSel}]
```

```
kslowMq
```

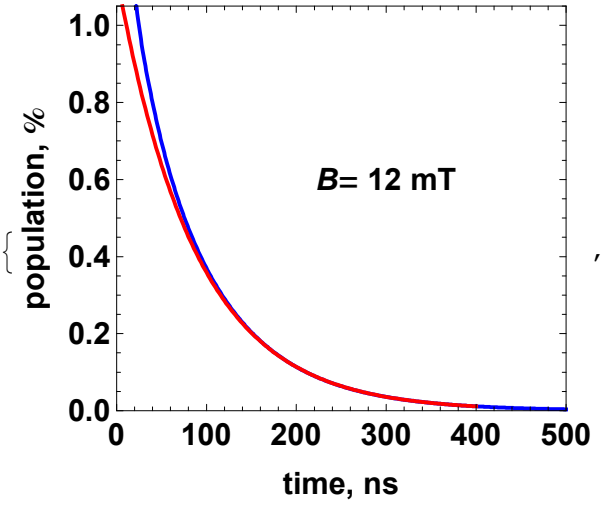
$$\{\{\{0, 1.0565\times10^{7}\}, \{2, 1.06843\times10^{7}\}, \{5, 1.11238\times10^{7}\}, \{7, 1.15653\times10^{7}\},$$
$$\{9, 1.16631\times10^{7}\}, \{10, 1.16251\times10^{7}\}, \{11, 1.15791\times10^{7}\}, \{12, 1.15032\times10^{7}\},$$
$$\{13, 1.13016\times10^{7}\}, \{15, 1.05916\times10^{7}\}, \{17, 9.96143\times10^{6}\}, \{20, 9.30117\times10^{6}\},$$
$$\{25, 8.63384\times10^{6}\}, \{30, 8.25649\times10^{6}\}, \{40, 7.88579\times10^{6}\}, \{50, 7.72113\times10^{6}\},$$
$$\{60, 7.63469\times10^{6}\}, \{80, 7.55131\times10^{6}\}, \{100, 7.51369\times10^{6}\}, \{200, 7.46457\times10^{6}\}\}\}$$

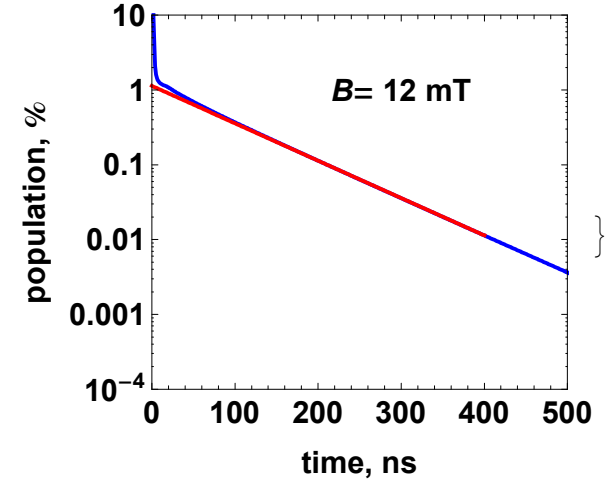
```
S1sim = Table[{t, AslowMq[[np, n, 2]] * Exp[-kslowMq[[np, n, 2]] / 10^9 * t]},
    {np, Np}, {n, nSel}, {t, 0, 400, 2}];

n = 6;
ListPlot[{S1pop225[[1, n]], S1sim[[1, n]]},
 PlotStyle → {{Thick, Blue}, {Thick, Red}, {Thick, Black}},
 PlotRange → {{0.0, 500}, {0.0, 2}}, Joined → True,
 BaseStyle -> {FontFamily → "Arial", FontWeight → "Bold", FontSize → 16},
 AspectRatio → 0.9, ImageSize → 400, Frame → True,
 FrameLabel → {"time, ns", "population, %"}]
```



```
n = 8;
{ListPlot[{S1pop225[[1, n]], S1sim[[1, n]]},
  PlotStyle → {{Thick, Blue}, {Thick, Red}, {Thick, Black},
    {Thick, DCyan, Dashed}, {Thick, Black, Dashed}, {Thick, DCyan, Dashed}},
  PlotRange → {{0.0, 500}, {0.0, 1.05}}, Joined → True,
  BaseStyle -> {FontFamily → "Arial", FontWeight → "Bold", FontSize → 16},
  AspectRatio → 0.9, ImageSize → 300, Frame → True,
  FrameLabel → {"time, ns", "population, %"},
  Epilog → Inset[StringJoin["B= ", ToString[FeldSel[[n]]], " mT"], {300, 0.6}]],
 ListLogPlot[{S1pop225[[1, n]], S1sim[[1, n]]},
  PlotStyle → {{Thick, Blue}, {Thick, Red}, {Thick, Black},
    {Thick, DCyan, Dashed}, {Thick, Black, Dashed}, {Thick, DCyan, Dashed}},
  PlotRange → {{0.0, 500}, {0.0001, 10}}, Joined → True,
  BaseStyle -> {FontFamily → "Arial", FontWeight → "Bold", FontSize → 16},
  AspectRatio → 0.9, ImageSize → 300, Frame → True,
  FrameLabel → {"time, ns", "population, %"}, Epilog →
   Inset[StringJoin["B= ", ToString[FeldSel[[n]]], " mT"], {300, Log[1]}]]}
```





==========
==========

scS1-model Auswertung k1CSSscl

```
Lsl[x_, xa_, xb_] := Log[x[[xa, 2]] / x[[xb, 2]]] / (x[[xb, 1]] - x[[xa, 1]])
LA[x_, xa_, xb_] := Exp[Log[x[[xa, 2]]] + Lsl[x, xa, xb] * x[[xa, 1]]]
k1CSSscl = ConstantArray[0, {Np, nSel, 2}];
A1CSSscl = ConstantArray[0, {Np, nSel, 2}];
Do[(
  m = Lsl[SRPvsB[[np, n]], 200, 400] // Chop;
  Amp = LA[SRPvsB[[np, n]], 200, 400] // Chop;
  A1CSSscl[[np, n]] = {FeldSel[[n]], Amp};
  k1CSSscl[[np, n]] = {FeldSel[[n]], 10^9 m}),
 {np, Np}, {n, nSel}]
```

```
A1CSSscl
```

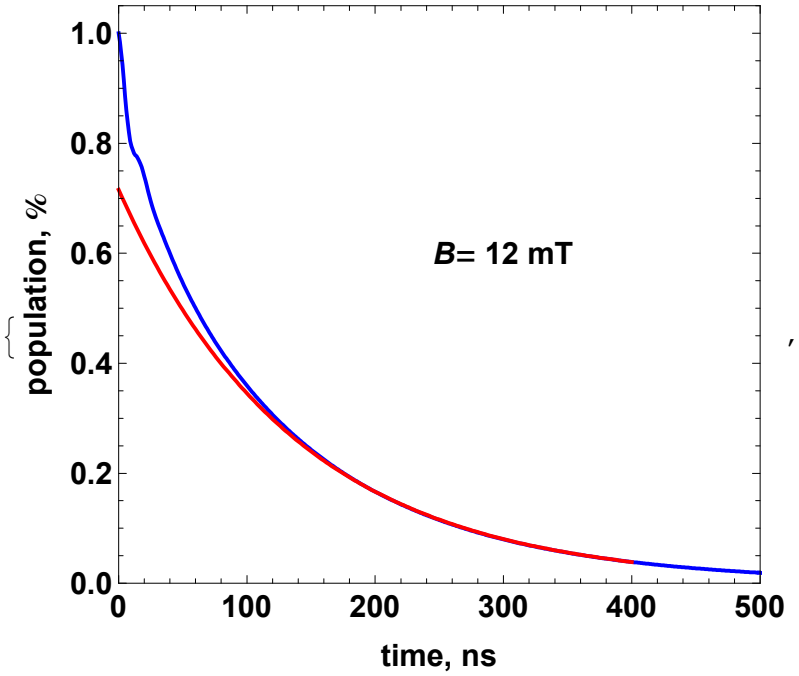
```
{{{0, 0.954289}, {2, 0.951984}, {5, 0.927123}, {7, 0.847984},
  {9, 0.63461}, {10, 0.588165}, {11, 0.613789}, {12, 0.715639},
  {13, 0.833851}, {15, 0.933431}, {17, 0.956702}, {20, 0.970022},
  {25, 0.979021}, {30, 0.982161}, {40, 0.983863}, {50, 0.984219},
  {60, 0.984319}, {80, 0.984366}, {100, 0.984372}, {200, 0.984367}}}
```

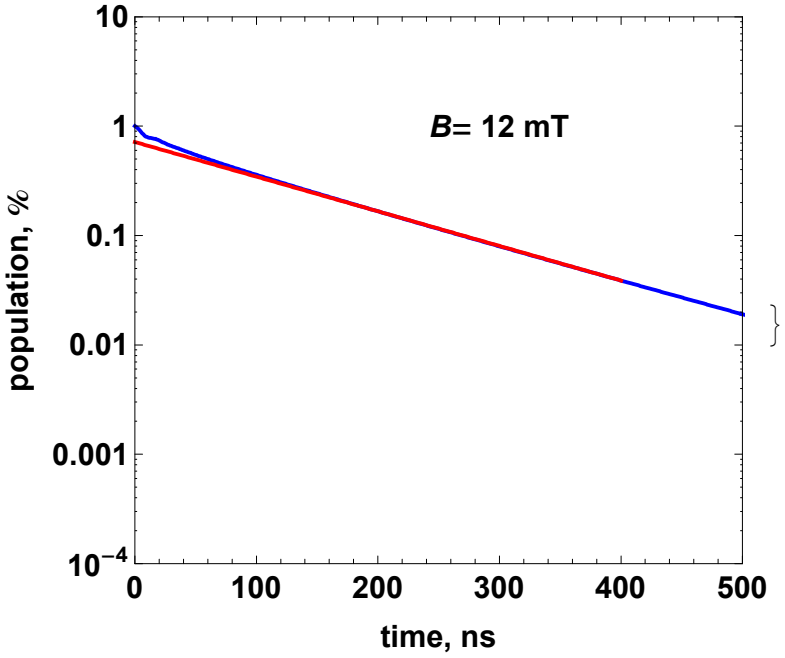
```
k1CSSscl
```

$$\left\{\left\{\left\{0, 5.94577\times10^{6}\right\}, \left\{2, 6.0736\times10^{6}\right\}, \left\{5, 6.63128\times10^{6}\right\}, \left\{7, 7.28531\times10^{6}\right\},\right.\right.$$
$$\left\{9, 7.42776\times10^{6}\right\}, \left\{10, 7.33649\times10^{6}\right\}, \left\{11, 7.31215\times10^{6}\right\}, \left\{12, 7.28945\times10^{6}\right\},$$
$$\left\{13, 7.01092\times10^{6}\right\}, \left\{15, 6.0341\times10^{6}\right\}, \left\{17, 5.27961\times10^{6}\right\}, \left\{20, 4.54211\times10^{6}\right\},$$
$$\left\{25, 3.82707\times10^{6}\right\}, \left\{30, 3.43261\times10^{6}\right\}, \left\{40, 3.0509\times10^{6}\right\}, \left\{50, 2.88301\times10^{6}\right\},$$
$$\left.\left.\left\{60, 2.79525\times10^{6}\right\}, \left\{80, 2.71083\times10^{6}\right\}, \left\{100, 2.67282\times10^{6}\right\}, \left\{200, 2.62324\times10^{6}\right\}\right\}\right\}$$

```
SCSSsclsim = Table[{t, A1CSSscl[[np, n, 2]] * Exp[-k1CSSscl[[np, n, 2]] / 10^9 * t]},
    {np, Np}, {n, nSel}, {t, 0, 400, 2}];

n = 8;
{ListPlot[{SRPvsB[[1, n]], SCSSsclsim[[1, n]]},
  PlotStyle → {{Thick, Blue}, {Thick, Red}, {Thick, Black},
    {Thick, DCyan, Dashed}, {Thick, Black, Dashed}, {Thick, DCyan, Dashed}},
  PlotRange → {{0.0, 500}, {0.0, 1.05}}, Joined → True,
  BaseStyle -> {FontFamily → "Arial", FontWeight → "Bold", FontSize → 16},
  AspectRatio → 0.9, ImageSize → 400, Frame → True,
  FrameLabel → {"time, ns", "population, %"},
  Epilog → Inset[StringJoin["B= ", ToString[FeldSel[[n]]], " mT"], {300, 0.6}]],
 ListLogPlot[{SRPvsB[[1, n]], SCSSsclsim[[1, n]]},
  PlotStyle → {{Thick, Blue}, {Thick, Red}, {Thick, Black},
    {Thick, DCyan, Dashed}, {Thick, Black, Dashed}, {Thick, DCyan, Dashed}},
  PlotRange → {{0.0, 500}, {0.0001, 10}}, Joined → True,
  BaseStyle -> {FontFamily → "Arial", FontWeight → "Bold", FontSize → 16},
  AspectRatio → 0.9, ImageSize → 400, Frame → True,
  FrameLabel → {"time, ns", "population, %"}, Epilog →
   Inset[StringJoin["B= ", ToString[FeldSel[[n]]], " mT"], {300, Log[1]}]]}
```





kdeph

0.

scS1-model Auswertung kCSSscl

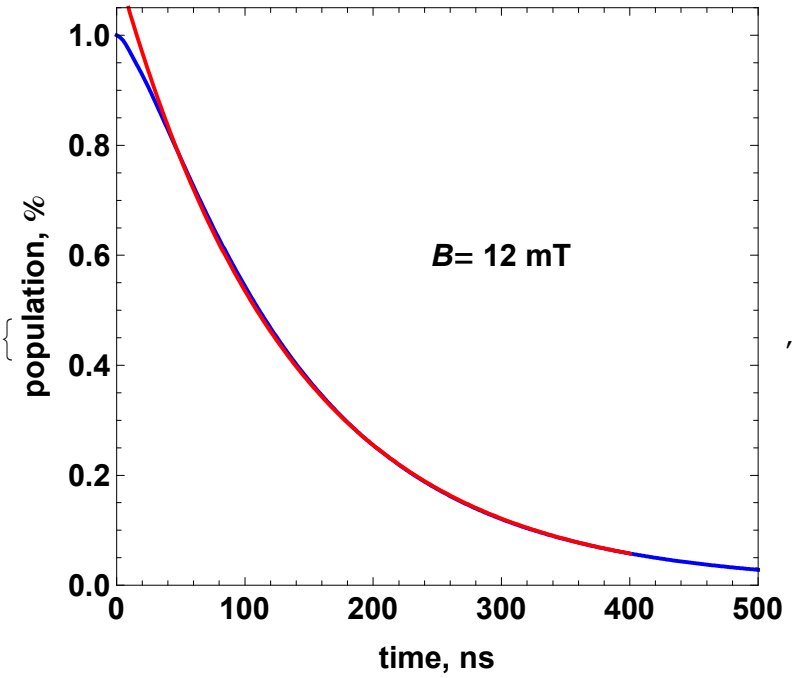
```
Lsl[x_, xa_, xb_] := Log[x[[xa, 2]] / x[[xb, 2]]] / (x[[xb, 1]] - x[[xa, 1]])
LA[x_, xa_, xb_] := Exp[Log[x[[xa, 2]]] + Lsl[x, xa, xb] * x[[xa, 1]]]
kCSSscl = ConstantArray[0, {Np, nSel, 2}];
ACSSscl = ConstantArray[0, {Np, nSel, 2}];
Do[(
  m = Lsl[RPvsB[[np, n]], 200, 400] // Chop;
  Amp = LA[RPvsB[[np, n]], 200, 400] // Chop;
  ACSSscl[[np, n]] = {FeldSel[[n]], Amp};
  kCSSscl[[np, n]] = {FeldSel[[n]], 10^9 m}),
 {np, Np}, {n, nSel}]
```

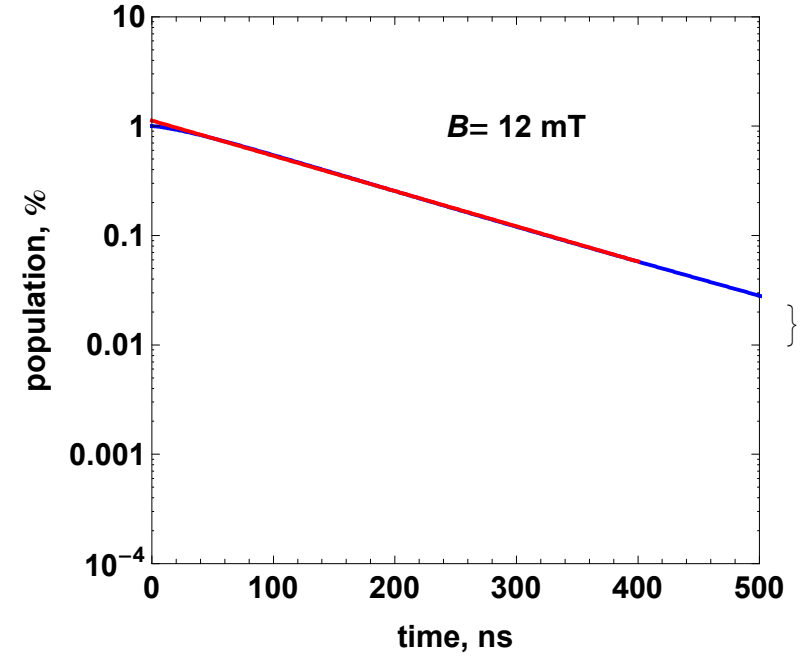
```
kCSSscl
```

$$\{\{\{0, 5.89933\times10^6\}, \{2, 6.02527\times10^6\}, \{5, 6.58402\times10^6\}, \{7, 7.2964\times10^6\},$$
$$\{9, 7.61971\times10^6\}, \{10, 7.52607\times10^6\}, \{11, 7.50077\times10^6\}, \{12, 7.41938\times10^6\},$$
$$\{13, 7.03683\times10^6\}, \{15, 5.99726\times10^6\}, \{17, 5.2482\times10^6\}, \{20, 4.51965\times10^6\},$$
$$\{25, 3.8116\times10^6\}, \{30, 3.42096\times10^6\}, \{40, 3.04328\times10^6\}, \{50, 2.87727\times10^6\},$$
$$\{60, 2.79051\times10^6\}, \{80, 2.70707\times10^6\}, \{100, 2.66949\times10^6\}, \{200, 2.62049\times10^6\}\}\}$$

```
CSSsclsim = Table[{t, ACSSscl[[np, n, 2]] * Exp[-kCSSscl[[np, n, 2]] / 10^9 * t]},
    {np, Np}, {n, nSel}, {t, 0, 400, 2}];
```

```
n = 8;
{ListPlot[{RPvsB[[1, n]], CSSsclsim[[1, n]]},
  PlotStyle → {{Thick, Blue}, {Thick, Red}, {Thick, Black},
    {Thick, DCyan, Dashed}, {Thick, Black, Dashed}, {Thick, DCyan, Dashed}},
  PlotRange → {{0.0, 500}, {0.0, 1.05}}, Joined → True,
  BaseStyle -> {FontFamily → "Arial", FontWeight → "Bold", FontSize → 16},
  AspectRatio → 0.9, ImageSize → 400, Frame → True,
  FrameLabel → {"time, ns", "population, %"},
  Epilog → Inset[StringJoin["B= ", ToString[FeldSel[[n]]], " mT"], {300, 0.6}]],
 ListLogPlot[{RPvsB[[1, n]], CSSsclsim[[1, n]]},
  PlotStyle → {{Thick, Blue}, {Thick, Red}, {Thick, Black},
    {Thick, DCyan, Dashed}, {Thick, Black, Dashed}, {Thick, DCyan, Dashed}},
  PlotRange → {{0.0, 500}, {0.0001, 10}}, Joined → True,
  BaseStyle -> {FontFamily → "Arial", FontWeight → "Bold", FontSize → 16},
  AspectRatio → 0.9, ImageSize → 400, Frame → True,
  FrameLabel → {"time, ns", "population, %"}, Epilog →
   Inset[StringJoin["B= ", ToString[FeldSel[[n]]], " mT"], {300, Log[1]}]]}
```





==========

==========

SCSS225

```
Lsl[x_, xa_, xb_] := Log[x[[xa, 2]] / x[[xb, 2]]] / (x[[xb, 1]] - x[[xa, 1]])
LA[x_, xa_, xb_] := Exp[Log[x[[xa, 2]]] + Lsl[x, xa, xb] * x[[xa, 1]]]
k1CSS = ConstantArray[0, {Np, nSel, 2}];
A1CSS = ConstantArray[0, {Np, nSel, 2}];
```

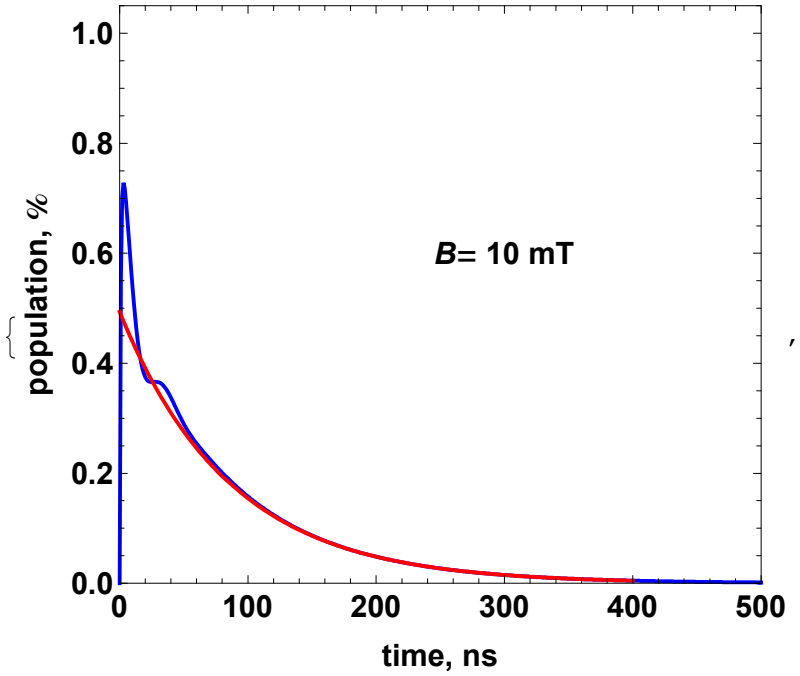
```
Do[(
  m = Lsl[SRPvsB225[[np, n]], 200, 400] // Chop;
  Amp = LA[SRPvsB225[[np, n]], 200, 400] // Chop;
  A1CSS[[np, n]] = {FeldSel[[n]], Amp};
  k1CSS[[np, n]] = {FeldSel[[n]], 10^9 m}),
 {np, Np}, {n, nSel}]
```

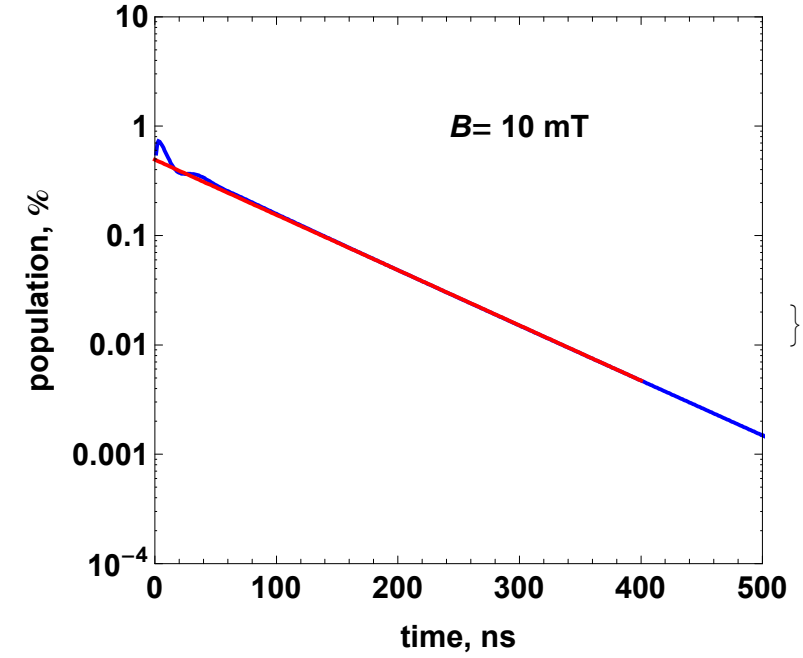
```
k1CSS
```

$$\{\{\{0, 1.05647\times10^{7}\}, \{2, 1.0684\times10^{7}\}, \{5, 1.11233\times10^{7}\}, \{7, 1.15645\times10^{7}\},$$
$$\{9, 1.16623\times10^{7}\}, \{10, 1.16244\times10^{7}\}, \{11, 1.15783\times10^{7}\}, \{12, 1.15024\times10^{7}\},$$
$$\{13, 1.13009\times10^{7}\}, \{15, 1.05913\times10^{7}\}, \{17, 9.96118\times10^{6}\}, \{20, 9.30097\times10^{6}\},$$
$$\{25, 8.63368\times10^{6}\}, \{30, 8.25635\times10^{6}\}, \{40, 7.88566\times10^{6}\}, \{50, 7.721\times10^{6}\},$$
$$\{60, 7.63456\times10^{6}\}, \{80, 7.55118\times10^{6}\}, \{100, 7.51356\times10^{6}\}, \{200, 7.46443\times10^{6}\}\}\}$$

```
SCSSsim = Table[{t, A1CSS[[np, n, 2]] * Exp[-k1CSS[[np, n, 2]] / 10^9 * t]},
    {np, Np}, {n, nSel}, {t, 0, 400, 2}];
```

```
n = 6;
{ListPlot[{sRPvsB225[[1, n]], SCSSsim[[1, n]]},
  PlotStyle → {{Thick, Blue}, {Thick, Red}, {Thick, Black},
    {Thick, DCyan, Dashed}, {Thick, Black, Dashed}, {Thick, DCyan, Dashed}},
  PlotRange → {{0.0, 500}, {0.0, 1.05}}, Joined → True,
  BaseStyle -> {FontFamily → "Arial", FontWeight → "Bold", FontSize → 16},
  AspectRatio → 0.9, ImageSize → 400, Frame → True,
  FrameLabel → {"time, ns", "population, %"},
  Epilog → Inset[StringJoin["B= ", ToString[FeldSel[[n]]], " mT"], {300, 0.6}]],
 ListLogPlot[{sRPvsB225[[1, n]], SCSSsim[[1, n]]},
  PlotStyle → {{Thick, Blue}, {Thick, Red}, {Thick, Black},
    {Thick, Cyan, Dashed}, {Thick, Black, Dashed}, {Thick, Cyan, Dashed}},
  PlotRange → {{0.0, 500}, {0.0001, 10}}, Joined → True,
  BaseStyle -> {FontFamily → "Arial", FontWeight → "Bold", FontSize → 16},
  AspectRatio → 0.9, ImageSize → 400, Frame → True,
  FrameLabel → {"time, ns", "population, %"}, Epilog →
   Inset[StringJoin["B= ", ToString[FeldSel[[n]]], " mT"], {300, Log[1]}]]}
```





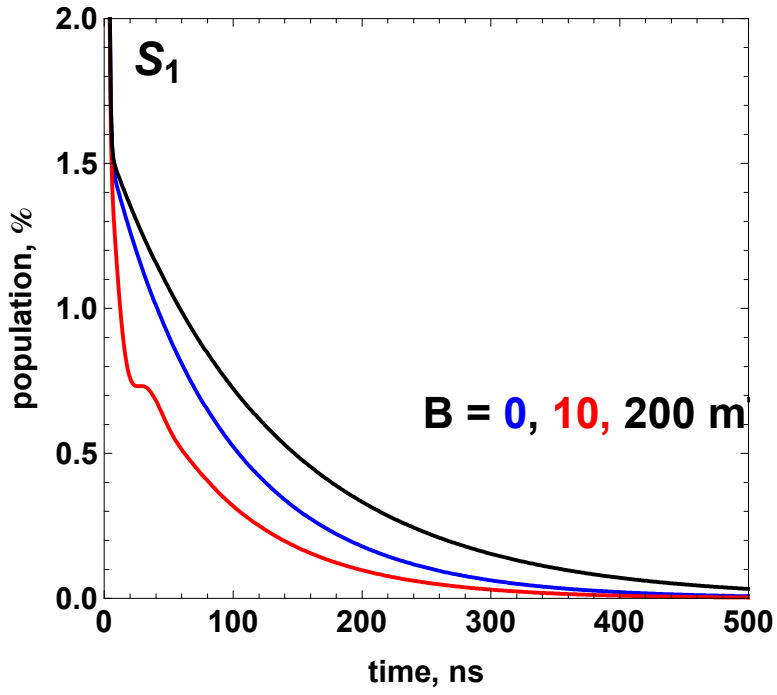
==========

SETS1 // TableForm

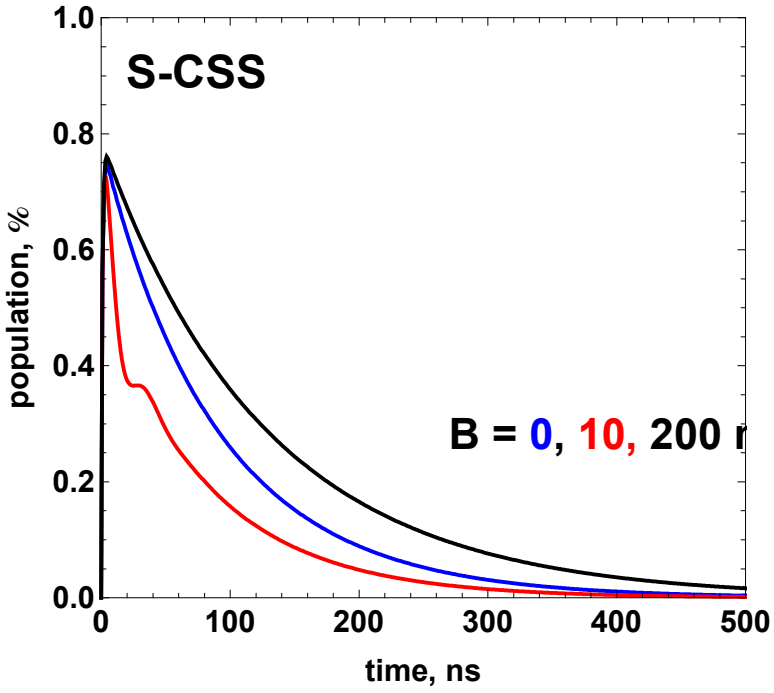
kCS	krCS	kf	ks	kt	k_{STD}	Tlong	τ	2J,G	ΔA,G	a,G
1.	0.025	0.25	0.001	0.02	0.1	∞	0.6	10.	15	10.

Diagram selection

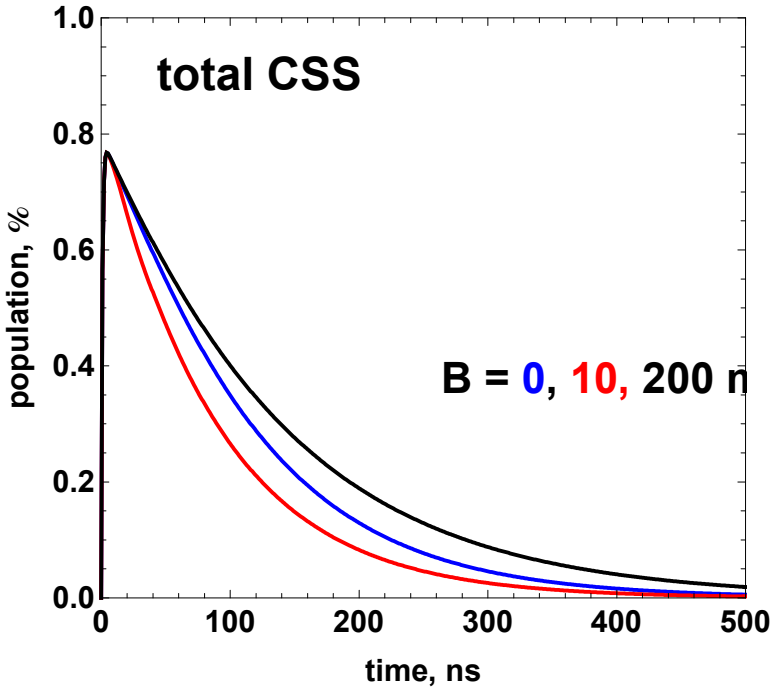
```
ListPlot[{S1pop225[[1, 1]], S1pop225[[1, 6]], S1pop225[[1, 16]]},
 PlotStyle → {{Thick, Blue}, {Thick, Red}, {Thick, Black}},
 PlotRange → {{0.0, 500}, {0.0, 2}}, Joined → True,
 BaseStyle -> {FontFamily → "Arial", FontWeight → "Bold", FontSize → 16},
 AspectRatio → 0.9, ImageSize → 400, Frame → True,
 FrameLabel → {"time, ns", "population, %"}]
```



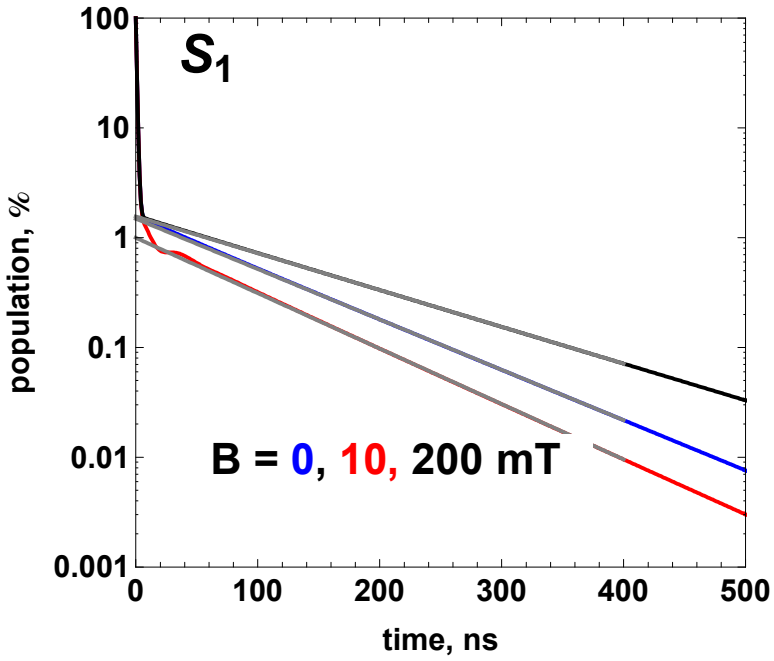

```
ListPlot[{SRPvsB225[[1, 1]], SRPvsB225[[1, 6]], SRPvsB225[[1, 16]]},
 PlotStyle → {{Thick, Blue}, {Thick, Red}, {Thick, Black}},
 PlotRange → {{0.0, 500}, {0.0, 1}}, Joined → True,
 BaseStyle -> {FontFamily → "Arial", FontWeight → "Bold", FontSize → 16},
 AspectRatio → 0.9, ImageSize → 400, Frame → True,
 FrameLabel → {"time, ns", "population, %"}]
```



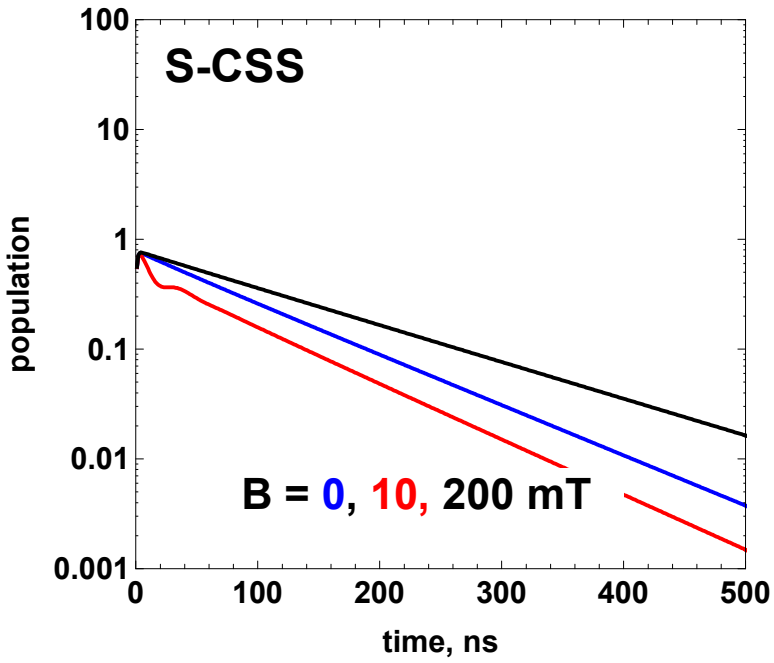

```
ListPlot[{RPvsB225[[1, 1]], RPvsB225[[1, 6]], RPvsB225[[1, 16]]},
 PlotStyle → {{Thick, Blue}, {Thick, Red}, {Thick, Black}},
 PlotRange → {{0.0, 500}, {0.0, 1}}, Joined → True,
 BaseStyle -> {FontFamily → "Arial", FontWeight → "Bold", FontSize → 16},
 AspectRatio → 0.9, ImageSize → 400, Frame → True,
 FrameLabel → {"time, ns", "population, %"}]
```



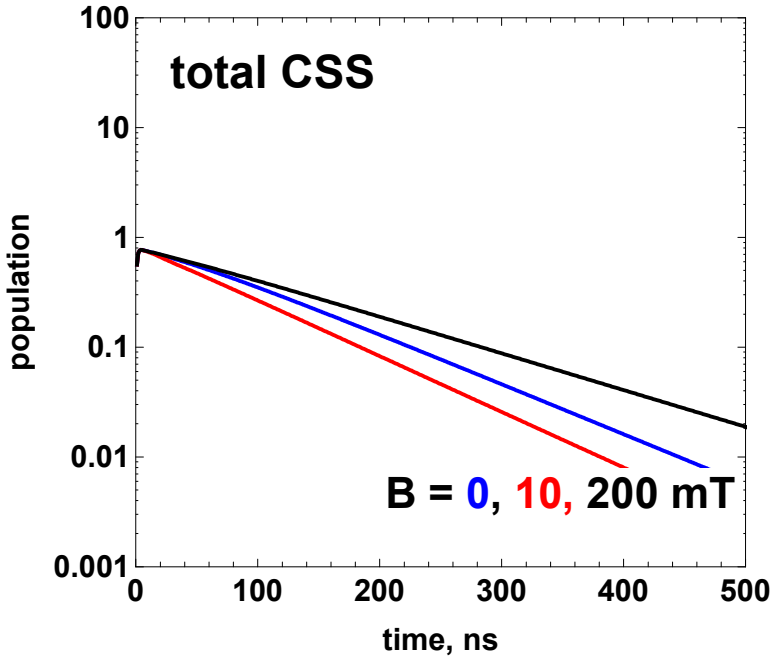
```
ListLogPlot[{S1pop225[[1, 1]], S1pop225[[1, 6]],
  S1pop225[[1, 16]], S1sim[[1, 1]], S1sim[[1, 6]], S1sim[[1, 16]]},
 PlotStyle → {{Thick, Blue}, {Thick, Red}, {Thick, Black},
   {Thick, Gray}, {Thick, Gray}, {Thick, Gray}},
 PlotRange → {{0.0, 500}, {0.001, 100}}, Joined → True,
 BaseStyle -> {FontFamily → "Arial", FontWeight → "Bold", FontSize → 16},
 AspectRatio → 0.9, ImageSize → 400, Frame → True,
 FrameLabel → {"time, ns", "population, %"}]
```




```
ListLogPlot[{SRPvsB225[[1, 1]], SRPvsB225[[1, 6]], SRPvsB225[[1, 16]]},
 PlotStyle → {{Thick, Blue}, {Thick, Red}, {Thick, Black}},
 PlotRange → {{0.0, 500}, {0.001, 100}}, Joined → True,
 BaseStyle -> {FontFamily → "Arial", FontWeight → "Bold", FontSize → 16},
 AspectRatio → 0.9, ImageSize → 400, Frame → True,
 FrameLabel → {"time, ns", "population"}]
```




```
ListLogPlot[{RPvsB225[[1, 1]], RPvsB225[[1, 6]], RPvsB225[[1, 16]]},
 PlotStyle → {{Thick, Blue}, {Thick, Red}, {Thick, Black}},
 PlotRange → {{0.0, 500}, {0.001, 100}}, Joined → True,
 BaseStyle -> {FontFamily → "Arial", FontWeight → "Bold", FontSize → 16},
 AspectRatio → 0.9, ImageSize → 400, Frame → True,
 FrameLabel → {"time, ns", "population"}]
```



kslowMq

$$\{\{\{0, 1.0565\times10^7\}, \{2, 1.06843\times10^7\}, \{5, 1.11238\times10^7\}, \{7, 1.15653\times10^7\}, \{9, 1.16631\times10^7\}, \{10, 1.16251\times10^7\}, \{11, 1.15791\times10^7\}, \{12, 1.15032\times10^7\}, \{13, 1.13016\times10^7\}, \{15, 1.05916\times10^7\}, \{17, 9.96143\times10^6\}, \{20, 9.30117\times10^6\}, \{25, 8.63384\times10^6\}, \{30, 8.25649\times10^6\}, \{40, 7.88579\times10^6\}, \{50, 7.72113\times10^6\}, \{60, 7.63469\times10^6\}, \{80, 7.55131\times10^6\}, \{100, 7.51369\times10^6\}, \{200, 7.46457\times10^6\}\}\}$$

SETS1 // TableForm

kCS	krCS	kf	ks	kt	k_{STD}	Tlong	τ	2J,G	ΔA,G	a,G
1.	0.025	0.25	0.001	0.02	0.1	∞	0.6	10.	15	10.

k1CSS

$$\{\{\{0, 1.05647\times10^7\}, \{2, 1.0684\times10^7\}, \{5, 1.11233\times10^7\}, \{7, 1.15645\times10^7\}, \{9, 1.16623\times10^7\}, \{10, 1.16244\times10^7\}, \{11, 1.15783\times10^7\}, \{12, 1.15024\times10^7\}, \{13, 1.13009\times10^7\}, \{15, 1.05913\times10^7\}, \{17, 9.96118\times10^6\}, \{20, 9.30097\times10^6\}, \{25, 8.63368\times10^6\}, \{30, 8.25635\times10^6\}, \{40, 7.88566\times10^6\}, \{50, 7.721\times10^6\}, \{60, 7.63456\times10^6\}, \{80, 7.55118\times10^6\}, \{100, 7.51356\times10^6\}, \{200, 7.46443\times10^6\}\}\}$$

kCSS

$$\{\{\{0, 1.04243\times10^7\}, \{2, 1.05383\times10^7\}, \{5, 1.09804\times10^7\}, \{7, 1.14919\times10^7\}, \{9, 1.1724\times10^7\}, \{10, 1.16817\times10^7\}, \{11, 1.16346\times10^7\}, \{12, 1.15266\times10^7\}, \{13, 1.12502\times10^7\}, \{15, 1.04755\times10^7\}, \{17, 9.85549\times10^6\}, \{20, 9.21646\times10^6\}, \{25, 8.57113\times10^6\}, \{30, 8.2066\times10^6\}, \{40, 7.84896\times10^6\}, \{50, 7.69023\times10^6\}, \{60, 7.60692\times10^6\}, \{80, 7.52656\times10^6\}, \{100, 7.49031\times10^6\}, \{200, 7.44296\times10^6\}\}\}$$

```
ListLinePlot[{kCSSscl[[1]], kslowMq[[1]]},
 PlotRange → {{-0.5, 61}, {2 * 10^6, 2 * 10^7}},
 BaseStyle → {FontFamily → "Arial", FontSize → 16, FontWeight → Bold},
 GridLines → Automatic, PlotStyle → {{Thick, Red}, {Thick, Blue},
   {Thickness[0.01], Red, Dashed}, {Thickness[0.01], Blue, Dashed}},
 AspectRatio → 0.8, Axes → False, Frame → True,
 FrameLabel → {{Style["kslow/s^-1", 20], None}, {"magnetic field/mT", None}},
 FrameTicks → {{Automatic, Automatic}, {Automatic, None}}, ImageSize → 500,
 Epilog → {PointSize[0.02], Cyan, Point[kslowMq[[1, 1 ;; 6]]], Blue,
   Point[kslowMq[[1, 7 ;; 16]]], Black, Point[k1CSS[[1]]], Red, Point[kCSS[[1]]]}]
```