In[1]:=
```
SetDirectory[NotebookDirectory[]];
```

$A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} B$ reaction network

Evaluate path integral to get pathway probability

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1. A general function for $\rho_{TRP}(\vec{\tau}_N \mid t = 0; PATH_N)$ for production of species A and B.

Gonna to use Mathematica double blank and pure function.

In[2]:=
```
(*Symbol comvert string to variable*)
(*With is kind of global, it will evaluate the expression at the end*)
(*Use ; at the end of each block*)
```

Final version, odd number N represents probability of pathway ending with species B;

even number N represents probability of pathway ending with species A.

In[3]:=
```
functionNv2[N_] :=
  Module[{Neven, Nodd, output}, (*Variables declaration→ local viriables*)
   Nodd = Quotient[N, 2] + Mod[N, 2];
   Neven = Quotient[N, 2];
   tlist = Table[StringJoin["t", IntegerString[i]], {i, 1, Neven + Nodd}];
   output = Product[
     (*With[{var=Symbol[todd[[i]]]},*)
     With[{},
      Evaluate[k1 * e^(-k1*Symbol[tlist[[2*i-1]]])]] (*With*)
     , {i, 1, Nodd}] (*Product*);
   For[j = 1, j ≤ Neven, j++,
    output *=
     With[{},
      Evaluate[k2 * e^(-k2*Symbol[tlist[[2*j]]])]] (*With*)
   ] (*For*);
   output *=
     If[Mod[N, 2] == 1, e^(-k2*(tf-Sum[Symbol[tlist[[i]]], {i, 1, N}])), e^(-k1*(tf-Sum[Symbol[tlist[[i]]], {i, 1, N}]))] // Simplify;

   (*Integral*)
   For[i = N, i > 1, i--,
    output = Integrate[output, {Symbol[tlist[[i]]], Symbol[tlist[[i - 1]]], tf}]
   ];
   If[N == 0, output = e^(-k1*tf), output = Integrate[output, {t1, 0, tf}]];
   Return[output];
  ](*FunctionNv2*);

(*Example*)
functionNv2[3]
```

Out[4]=
$$\frac{e^{-k_1 t_f} k_1^2 k_2 \left(\mathrm{Sinh}\left[\left(k_1 - k_2\right) t_f\right] + \left(-k_1 + k_2\right) t_f\right)}{\left(k_1 - k_2\right)^3}$$

In[5]:=
```
functionNv2[0]
```

Out[5]= $e^{-k_1 t_f}$

Fist N terms of pathway ending with species B.

In[6]:=
```
probB = Table[functionNv2[2 * i + 1], {i, 0, 5 - 1}];
probB
```

Out[7]=

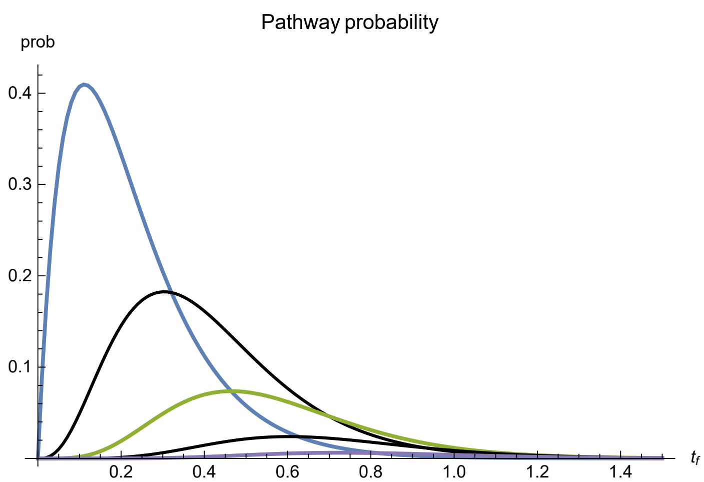
$$\left\{-\frac{\left(e^{-k_1 t_f}-e^{-k_2 t_f}\right) k_1}{k_1-k_2},\ \frac{e^{-k_1 t_f} k_1^2 k_2 \left(\mathrm{Sinh}\left[\left(k_1-k_2\right) t_f\right]+\left(-k_1+k_2\right) t_f\right)}{\left(k_1-k_2\right)^3},\ \frac{1}{6\left(k_1-k_2\right)^5} e^{\frac{1}{2}\left(-3 k_1+k_2\right) t_f} k_1^3 k_2^2 \left(9\,\mathrm{Sinh}\left[\frac{1}{2}\left(k_1-k_2\right) t_f\right]+\mathrm{Sinh}\left[\frac{3}{2}\left(k_1-k_2\right) t_f\right]+6\,\mathrm{Cosh}\left[\frac{1}{2}\left(k_1-k_2\right) t_f\right]\left(-k_1+k_2\right) t_f\right),\right.$$

$$-\frac{1}{72\left(k_1-k_2\right)^7} e^{\left(-2 k_1+k_2\right) t_f} k_1^4 k_2^3 \left(-28\,\mathrm{Sinh}\left[\left(k_1-k_2\right) t_f\right]-\mathrm{Sinh}\left[2\left(k_1-k_2\right) t_f\right]+6\left(3+2\,\mathrm{Cosh}\left[\left(k_1-k_2\right) t_f\right]\right)\left(k_1-k_2\right) t_f\right),$$

$$\left.-\frac{1}{8640\left(k_1-k_2\right)^9} e^{-\left(5 k_1+k_2\right) t_f} k_1^5 k_2^4 \left(-3 e^{5 k_1 t_f}+3 e^{5 k_2 t_f}-175 e^{\left(4 k_1+k_2\right) t_f}-300 e^{\left(3 k_1+2 k_2\right) t_f}+300 e^{\left(2 k_1+3 k_2\right) t_f}+175 e^{\left(k_1+4 k_2\right) t_f}+60\left(e^{\left(4 k_1+k_2\right) t_f}+6 e^{\left(3 k_1+2 k_2\right) t_f}+6 e^{\left(2 k_1+3 k_2\right) t_f}+e^{\left(k_1+4 k_2\right) t_f}\right) k_1 t_f-60\left(e^{\left(4 k_1+k_2\right) t_f}+6 e^{\left(3 k_1+2 k_2\right) t_f}+6 e^{\left(2 k_1+3 k_2\right) t_f}+e^{\left(k_1+4 k_2\right) t_f}\right) k_2 t_f\right)\right\}$$

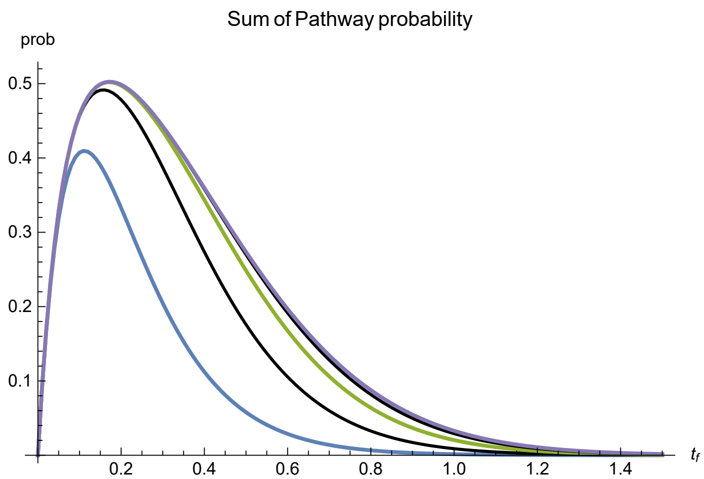
In[8]:=
```
tfinal = 1.5;
PointsB = Table[Table[{x, probB[[i]] /. {k₁ → 10.0, k₂ → 8.0, t_f → x} // Evaluate},
    {x, 0, tfinal, 0.01}], {i, 1, Length[probB]}];
ListLinePlot[PointsB, PlotLabel → HoldForm[Pathway probability],
 AxesLabel → {HoldForm[t_f], prob}, PlotStyle → {Thick, Black}, PlotRange → All]
```

Out[9]=



In[10]:=
```
tfinal = 1.5;
PointsBC =
 Table[Table[{x, Sum[probB[[j]], {j, 1, i}] /. {k1 → 10.0, k2 → 8.0, tf → x} // Evaluate},
   {x, 0, tfinal, 0.01}], {i, 1, Length[probB]}];
ListLinePlot[PointsBC, PlotLabel → HoldForm[Sum of Pathway probability],
 AxesLabel → {HoldForm[tf], prob}, PlotStyle → {Thick, Black}, PlotRange → All]
```

Out[11]=



Taylor expansion.

In[12]:=
```
probBTaylor = Table[Series[probB[[i]], {tf, 0, 9}], {i, 1, Length[probB]}];
probBTaylor
```

Out[13]=

$$\Big\{k_1 t_f - \frac{1}{2}\left(k_1\left(k_1+k_2\right)\right) t_f^2 + \frac{1}{6} k_1\left(k_1^2+k_1 k_2+k_2^2\right) t_f^3 + \frac{k_1\left(-k_1^4+k_2^4\right) t_f^4}{24\left(k_1-k_2\right)} + \frac{k_1\left(k_1^5-k_2^5\right) t_f^5}{120\left(k_1-k_2\right)} + \frac{k_1\left(-k_1^6+k_2^6\right) t_f^6}{720\left(k_1-k_2\right)} + \frac{k_1\left(k_1^7-k_2^7\right) t_f^7}{5040\left(k_1-k_2\right)} + \frac{k_1\left(-k_1^8+k_2^8\right) t_f^8}{40320\left(k_1-k_2\right)} + \frac{k_1\left(k_1^9-k_2^9\right) t_f^9}{362880\left(k_1-k_2\right)} + O[t_f]^{10},$$

$$\frac{1}{6} k_1^2 k_2 t_f^3 - \frac{1}{6}\left(k_1^3 k_2\right) t_f^4 + \frac{1}{120} k_1^2 k_2\left(11 k_1^2 - 2 k_1 k_2 + k_2^2\right) t_f^5 - \frac{1}{360}\left(k_1^3 k_2\left(13 k_1^2 - 6 k_1 k_2 + 3 k_2^2\right)\right) t_f^6 + \frac{k_1^2 k_2\left(57 k_1^4 - 46 k_1^3 k_2 + 27 k_1^2 k_2^2 - 4 k_1 k_2^3 + k_2^4\right) t_f^7}{5040} - \frac{\left(k_1^3 k_2\left(15 k_1^4 - 18 k_1^3 k_2 + 13 k_1^2 k_2^2 - 4 k_1 k_2^3 + k_2^4\right)\right) t_f^8}{5040} + \frac{1}{362880} k_1^2 k_2\left(247 k_1^6 - 402 k_1^5 k_2 + 357 k_1^4 k_2^2 - 164 k_1^3 k_2^3 + 51 k_1^2 k_2^4 - 6 k_1 k_2^5 + k_2^6\right) t_f^9 + O[t_f]^{10},$$

$$\frac{1}{120} k_1^3 k_2^2 t_f^5 + \frac{1}{240} k_1^3 k_2^2\left(-3 k_1 + k_2\right) t_f^6 + \frac{k_1^3 k_2^2\left(50 k_1^2 - 37 k_1 k_2 + 8 k_2^2\right) t_f^7}{5040} - \frac{\left(k_1^3 k_2^2\left(111 k_1^3 - 133 k_1^2 k_2 + 59 k_1 k_2^2 - 9 k_2^3\right)\right) t_f^8}{20160} + \frac{k_1^3 k_2^2\left(289 k_1^4 - 490 k_1^3 k_2 + 336 k_1^2 k_2^2 - 106 k_1 k_2^3 + 13 k_2^4\right) t_f^9}{120960} + O[t_f]^{10},$$

$$\frac{k_1^4 k_2^3 t_f^7}{5040} + \frac{k_1^4 k_2^3\left(-2 k_1 + k_2\right) t_f^8}{5040} + \frac{k_1^4 k_2^3\left(25 k_1^2 - 26 k_1 k_2 + 7 k_2^2\right) t_f^9}{60480} + O[t_f]^{10},\ \frac{k_1^5 k_2^4 t_f^9}{362880} + O[t_f]^{10}\Big\}$$

Compare pathway result with ODEs solution

In[14]:=
$$A = \frac{k_2}{k_1 + k_2} + \frac{k_1}{k_1 + k_2} e^{-(k_1+k_2)\, t_f};$$
$$B = \frac{k_1}{k_1 + k_2} \left(1 - e^{-(k_1+k_2)\, t_f}\right);$$

```
TaylorA = Series[A, {tf, 0, 9}] // Simplify
TaylorB = Series[B, {tf, 0, 9}] // Simplify
(*LaurentA=Series[A/.tf→1/t,{t,0,10}]*)
```

Out[16]=
$$1 - k_1 t_f + \frac{1}{2} k_1 (k_1 + k_2)\, t_f^2 - \frac{1}{6} \left(k_1 (k_1 + k_2)^2\right) t_f^3 + \frac{1}{24} k_1 (k_1 + k_2)^3\, t_f^4 - \frac{1}{120} \left(k_1 (k_1 + k_2)^4\right) t_f^5 + \frac{1}{720} k_1 (k_1 + k_2)^5\, t_f^6 - \frac{\left(k_1 (k_1 + k_2)^6\right) t_f^7}{5040} + \frac{k_1 (k_1 + k_2)^7\, t_f^8}{40\,320} - \frac{\left(k_1 (k_1 + k_2)^8\right) t_f^9}{362\,880} + O[t_f]^{10}$$

Out[17]=
$$k_1 t_f - \frac{1}{2} \left(k_1 (k_1 + k_2)\right) t_f^2 + \frac{1}{6} k_1 (k_1 + k_2)^2\, t_f^3 - \frac{1}{24} \left(k_1 (k_1 + k_2)^3\right) t_f^4 + \frac{1}{120} k_1 (k_1 + k_2)^4\, t_f^5 - \frac{1}{720} \left(k_1 (k_1 + k_2)^5\right) t_f^6 + \frac{k_1 (k_1 + k_2)^6\, t_f^7}{5040} - \frac{\left(k_1 (k_1 + k_2)^7\right) t_f^8}{40\,320} + \frac{k_1 (k_1 + k_2)^8\, t_f^9}{362\,880} + O[t_f]^{10}$$

In[18]:=
```
k1 = 10.0; k2 = 8.0; tfinal = 0.5
PointsAInit = Table[{x, A /. tf → x // Evaluate}, {x, 0, tfinal, 0.01}];
PointsBInit = Table[{x, B /. tf → x // Evaluate}, {x, 0, tfinal, 0.01}];
ListLinePlot[{PointsAInit, PointsBInit}, PlotLabel → HoldForm[Pathway probability],
 AxesLabel → {HoldForm[tf], prob}, PlotStyle → {Thick, Black}, PlotRange → All]
```

Out[18]= 0.5

Out[20]=