

In[1]:= w21 = w; w12 = 0;

(\* States are 11, 12, 22, 1|2. \*)

$$Q = \begin{pmatrix} -2 w_{21} - cA & 2 w_{21} & 0 & cA \\ w_{12} & -w_{21} - w_{12} & w_{21} & 0 \\ 0 & 2 w_{12} & -2 w_{12} - cC & cC \\ 0 & 0 & 0 & 0 \end{pmatrix};$$

EigenRoot = Eigenvalues [Q]

U = Transpose [Eigenvectors [Q] ];

V = Simplify [Inverse [U] ];

Simplify [U.V] ;

Ptau = Simplify [U.DiagonalMatrix [Exp [EigenRoot \* tauAB] ] .V] ;

Ptau[[1]]

P1 = Ptau[[1, 1]]; P2 = Ptau[[1, 2]]; P3 = Ptau[[1, 3]]; P4 = Ptau[[1, 4]];

P1 / 3 + P2 \* Exp [-2 / thetaAB \* (tauABC - tauAB) ] / 3  
+ P3 \* (1 - 2 / 3 \* Exp [-2 (tauABC - tauAB) / thetaC] ) + P4

Out[3]= {0, -cC, -cA - 2 w, -w}

$$\text{Out[8]} = \left\{ e^{-\tau_{AB}(cA+2w)}, -\frac{2 e^{-\tau_{AB} w} (-1 + e^{-\tau_{AB}(cA+w)}) w}{cA + w}, \right. \\ \left. \frac{2 w^2 (e^{-\tau_{AB}(cA+2w)} (cC - w) - e^{-cC \tau_{AB}} (cA + w) + e^{-\tau_{AB} w} (cA - cC + 2 w))}{(cC - w) (cA + w) (cA - cC + 2 w)}, \right. \\ \left. 1 - \frac{2 e^{-cC \tau_{AB}} w^2}{(-cA + cC - 2 w) (cC - w)} - \frac{2 cC e^{-\tau_{AB} w} w}{(cC - w) (cA + w)} - \frac{e^{-\tau_{AB}(cA+2w)} (cA^2 + cC w + cA (-cC + w))}{(cA + w) (cA - cC + 2 w)} \right\}$$

Out[10]=

$$\frac{1}{3} e^{-\tau_{AB}(cA+2w)} - \frac{2 e^{-\frac{2(-\tau_{AB}+\tau_{ABC})}{\theta_{AB}}-\tau_{AB} w} (-1 + e^{-\tau_{AB}(cA+w)}) w}{3 (cA + w)}$$

Out[11]=

$$1 - \frac{2 e^{-cC \tau_{AB}} w^2}{(-cA + cC - 2 w) (cC - w)} - \frac{2 cC e^{-\tau_{AB} w} w}{(cC - w) (cA + w)} - \frac{e^{-\tau_{AB}(cA+2w)} (cA^2 + cC w + cA (-cC + w))}{(cA + w) (cA - cC + 2 w)} + \\ \frac{2 \left( 1 - \frac{2}{3} e^{-\frac{2(-\tau_{AB}+\tau_{ABC})}{\theta_{AB}}} \right) w^2 (e^{-\tau_{AB}(cA+2w)} (cC - w) - e^{-cC \tau_{AB}} (cA + w) + e^{-\tau_{AB} w} (cA - cC + 2 w))}{(cC - w) (cA + w) (cA - cC + 2 w)}$$

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In[12]:= gdiJ[MCA_, tauABC_, tauAB_, thetaA_, thetaC_, thetaAB_] := Block[{cA, cC, w},
  cA = 2 / thetaA; cC = 2 / thetaC; w = 4 MCA / thetaA;
  P1 = e-tauAB (cA+2 w);
  P2 = -  $\frac{2 e^{-\tau_{AB} w} (-1 + e^{-\tau_{AB} (cA+w)}) w}{cA + w}$ ;
  P3 =  $\frac{2 w^2 (e^{-\tau_{AB} (cA+2 w)} (cC - w) - e^{-cC \tau_{AB}} (cA + w) + e^{-\tau_{AB} w} (cA - cC + 2 w))}{(cC - w) (cA + w) (cA - cC + 2 w)}$ ;
  P4 = 1 - P1 - P2 - P3;
  (* Print[{P1,P2,P3,P4}]; *)
  PG1 = P1 / 3 + P2 * Exp[-2 / thetaAB * (tauABC - tauAB)] / 3 +
    P3 * (1 - 2 / 3 * Exp[-2 (tauABC - tauAB) / thetaC]) + P4;
  (PG1 - 1 / 3) * (3 / 2)
];

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P4gdi[MCA_, tauABC_, tauAB_, thetaA_, thetaC_, thetaAB_] := Block[{cA, cC, w},
  cA = 2 / thetaA; cC = 2 / thetaC; w = 4 MCA / thetaA;
  P1 = e-tauAB (cA+2 w);
  P2 = -  $\frac{2 e^{-\tau_{AB} w} (-1 + e^{-\tau_{AB} (cA+w)}) w}{cA + w}$ ;
  P3 =  $\frac{2 w^2 (e^{-\tau_{AB} (cA+2 w)} (cC - w) - e^{-cC \tau_{AB}} (cA + w) + e^{-\tau_{AB} w} (cA - cC + 2 w))}{(cC - w) (cA + w) (cA - cC + 2 w)}$ ;
  P4 = 1 - P1 - P2 - P3
];

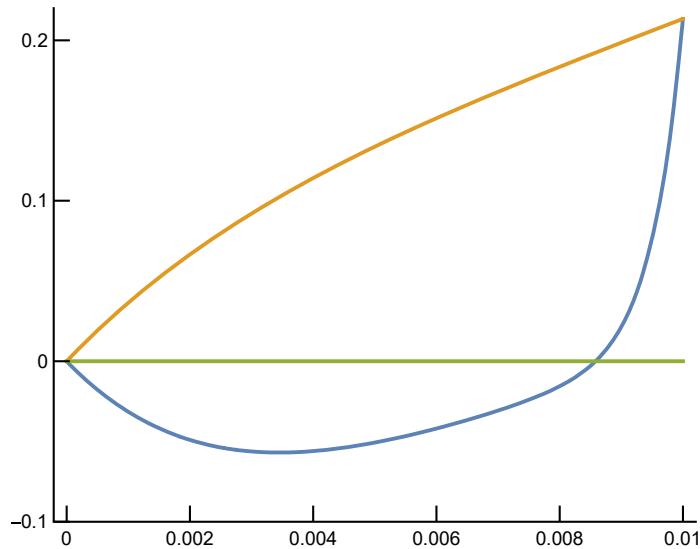
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In[*]:= MCA = 1; tauABC = 0.01;
tauAB = 0.005;
thetaA = 0.05; thetaC = 0.05; thetaAB = 0.001;
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```
Plot[{gdiJ[MCA, tauABC, tauAB, thetaA, thetaC, thetaAB],
P4gdi[MCA, tauABC, tauAB, thetaA, thetaC, thetaAB], 0},
{tauAB, 0, tauABC}, Frame → {{True, False}, {True, False}},
FrameStyle → Directive[AbsoluteThickness[Medium], Black, 10],
FrameTicks → {{{0, 0, .025}, {0.002, 0.002, .025}, {0.004, 0.004, .025},
{0.006, 0.006, .025}, {0.008, 0.008, .025}, {0.01, 0.01, .025}},
{{-0.1, -0.1, .025}, {0, 0, .025}, {0.1, 0.1, .025}, {0.2, 0.2, .025}}},
PlotRange → {-0.1, 0.22}, AxesOrigin → {0, -0.1}, AspectRatio → .8]
```

```
Plot[{gdiJ[MCA, tauABC, tauAB, thetaA, thetaC, thetaAB],
P4gdi[MCA, tauABC, tauAB, thetaA, thetaC, thetaAB], 0},
{MCA, 0, 2}, Frame → {{True, False}, {True, False}},
FrameStyle → Directive[AbsoluteThickness[Medium], Black, 12], FrameTicks →
{{{0, 0, .025}, {0.5, 0.5, .025}, {1, 1, .025}, {1.5, 1.5, .025}, {2, 2, .025}},
{{-0.1, " ", .025}, {0, "", .025}, {0.1, " ", .025}, {0.2, " ", .025}}},
PlotRange → {-0.1, 0.22}, AxesOrigin → {0, -0.1}, AspectRatio → .8]
```

Out[\*]=



Out[\*]=

