

In[1]:= **Clear**[g, V]

In[2]:= **g_{xy}**[x_, y_] := (y - x) / L
g_{yx}[x_, y_] := 1 + (y - x) / L

In[4]:= **V**[x_] := **Piecewise**[{{ ΔV x / (a L), x < a L}, { ΔV (L - x) / ((1 - a) L), x ≥ a L}}]

In[5]:= **Z**[β_] := L / (β ΔV) (1 - **Exp**[-β ΔV])

In[6]:= **inner**[f_] := **Integrate**[g_{yx}[x, y] f[y], {y, 0, x}, **Assumptions** → x > 0] +
Integrate[g_{xy}[x, y] f[y], {y, x, L}, **Assumptions** → x < L]

In[7]:= **full**[f_, g_] := **Integrate**[f[x] **inner**[g], {x, 0, L}, **Assumptions** → L > 0]

In[8]:= **fVv** = **Simplify**[**full**[**Exp**[β V[#]] &, **Exp**[-β V[#]] &],
Assumptions → L > 0 && 0 < a < 1 && ΔV > 0 && β > 0]

$$\text{Out[8]} = \frac{1}{\beta^3 \Delta V^3} e^{-\frac{a \beta \Delta V}{-1+a}} L^2 \left(-2 e^{\left(2 + \frac{1}{-1+a}\right) \beta \Delta V} + 5 a e^{\left(2 + \frac{1}{-1+a}\right) \beta \Delta V} - 3 a^2 e^{\left(2 + \frac{1}{-1+a}\right) \beta \Delta V} - 2 e^{\frac{\beta \Delta V}{-1+a}} + 5 a e^{\frac{\beta \Delta V}{-1+a}} - 3 a^2 e^{\frac{\beta \Delta V}{-1+a}} + 4 e^{\frac{a \beta \Delta V}{-1+a}} - \right. \\ \left. 8 a e^{\frac{a \beta \Delta V}{-1+a}} + e^{\left(2 + \frac{1}{-1+a}\right) \beta \Delta V} \beta \Delta V - 2 a e^{\left(2 + \frac{1}{-1+a}\right) \beta \Delta V} \beta \Delta V + a^2 e^{\left(2 + \frac{1}{-1+a}\right) \beta \Delta V} \beta \Delta V + \right. \\ \left. a e^{\frac{\beta \Delta V}{-1+a}} \beta \Delta V - a^2 e^{\frac{\beta \Delta V}{-1+a}} \beta \Delta V - e^{\frac{a \beta \Delta V}{-1+a}} \beta \Delta V + e^{\frac{a \beta \Delta V}{-1+a}} \beta^2 \Delta V^2 - 2 a e^{\frac{a \beta \Delta V}{-1+a}} \beta^2 \Delta V^2 + \right. \\ \left. a e^{\frac{a \beta \Delta V}{-1+a}} (-2 + 6 a + \beta \Delta V) \cosh[\beta \Delta V] - a (-1 + 2 a) e^{\frac{a \beta \Delta V}{-1+a}} \beta \Delta V \sinh[\beta \Delta V] \right)$$

In[9]:= **fVc** = **Simplify**[**full**[**Exp**[β V[#]] &, **Exp**[-β c V[#]] &],
Assumptions → L > 0 && 0 < a < 1 && ΔV > 0 && β > 0 && 0 < c < 1]

$$- \frac{1}{(-1+c) c^2 \beta^3 \Delta V^3} e^{-\frac{(1-2c+a(-1+3c)) \beta \Delta V}{-1+a}} L^2 \left((-1+c) e^{\frac{(-2+3a)c \beta \Delta V}{-1+a}} (1+c-c \beta \Delta V+a(-2+c(-2+\beta \Delta V))) - \right. \\ \left. e^{\frac{(-1+2a)c \beta \Delta V}{-1+a}} (-1+c^2(1-\beta \Delta V)+a(1+c)(2+c(-2+\beta \Delta V))) + \right. \\ \left. e^{\frac{(1-2c+a(-1+3c)) \beta \Delta V}{-1+a}} (1-c^2-c \beta \Delta V+a(1+c)(-2+c(2+\beta \Delta V))) - \right. \\ \left. (-1+c) e^{\left(-1+\left(2+\frac{1}{-1+a}\right)c\right) \beta \Delta V} (-1-c+a(2+c(2+\beta \Delta V))) \right)$$

**j1 = -Simplify[(fVc / (Z[β c] Z[-β]) - fVv / (Z[β] Z[-β])),
Assumptions → L > 0 && 0 < a < 1 && ΔV > 0 && β > 0 && 0 < c < 1]**

$$\frac{1}{(-1 + e^{\beta \Delta V}) \beta \Delta V} \left(\frac{1}{-1 + e^{\beta \Delta V}} (-2 + e^{2\beta \Delta V} (-2 + \beta \Delta V) + e^{\beta \Delta V} (4 - \beta \Delta V + \beta^2 \Delta V^2)) + \right. \\ \left. a (4 + \beta \Delta V + e^{2\beta \Delta V} (4 - \beta \Delta V) - 2 e^{\beta \Delta V} (4 + \beta^2 \Delta V^2)) \right) + \frac{1}{(-1 + c) c (1 - e^{-c \beta \Delta V})} \\ e^{-\frac{(1-2c+a)(-1+3c)\beta \Delta V}{-1+a}} \left((-1 + c) e^{\frac{(-2+3a)c\beta \Delta V}{-1+a}} (1 + c - c \beta \Delta V + a (-2 + c (-2 + \beta \Delta V))) - \right. \\ e^{\frac{(-1+2a)c\beta \Delta V}{-1+a}} (-1 + c^2 (1 - \beta \Delta V) + a (1 + c) (2 + c (-2 + \beta \Delta V))) + \\ \left. e^{\frac{(1-2c+a)(-1+3c)\beta \Delta V}{-1+a}} (1 - c^2 - c \beta \Delta V + a (1 + c) (-2 + c (2 + \beta \Delta V))) - \right. \\ \left. (-1 + c) e^{(-1 + (2 + \frac{1}{-1+a})c) \beta \Delta V} (-1 - c + a (2 + c (2 + \beta \Delta V))) \right) \Bigg)$$

**fcv = Simplify[full[Exp[β c V[#]] &, Exp[-β V[#]] &],
Assumptions → L > 0 && 0 < a < 1 && ΔV > 0 && β > 0 && 0 < c < 1]**

$$- \frac{1}{(-1 + c) c^2 \beta^3 \Delta V^3} e^{-\frac{(-2+2a+c)\beta \Delta V}{-1+a}} L^2 \left((-1 + c) e^{\frac{(-2+a)(2+c)\beta \Delta V}{-1+a}} (1 + c - c \beta \Delta V + a (-2 + c (-2 + \beta \Delta V))) - \right. \\ e^{\frac{(-2+2a+c)\beta \Delta V}{-1+a}} (-1 + c^2 (1 - \beta \Delta V) + a (1 + c) (2 + c (-2 + \beta \Delta V))) + \\ e^{\frac{(-1+a+c)\beta \Delta V}{-1+a}} (1 - c^2 - c \beta \Delta V + a (1 + c) (-2 + c (2 + \beta \Delta V))) - \\ \left. (-1 + c) e^{(1 + \frac{c}{-1+a}) \beta \Delta V} (-1 - c + a (2 + c (2 + \beta \Delta V))) \right)$$

**fcc = Simplify[full[Exp[β c V[#]] &, Exp[-β c V[#]] &],
Assumptions → L > 0 && 0 < a < 1 && ΔV > 0 && β > 0 && 0 < c < 1]**

$$\frac{1}{c^3 \beta^3 \Delta V^3} e^{-\frac{(-2+3a)c\beta \Delta V}{-1+a}} L^2 \left(e^{\frac{(-3+4a)c\beta \Delta V}{-1+a}} (-2 + c \beta \Delta V + a (4 - c \beta \Delta V)) + e^{(1 + \frac{a}{-1+a})c\beta \Delta V} (-2 + a (4 + c \beta \Delta V)) + \right. \\ \left. e^{\frac{(-2+3a)c\beta \Delta V}{-1+a}} (4 - c \beta \Delta V + c^2 \beta^2 \Delta V^2 - 2a (4 + c^2 \beta^2 \Delta V^2)) \right)$$

**jc = -FullSimplify[(fcv / (Z[-β c] Z[β]) - fcc / (Z[c β] Z[-c β])),
Assumptions → L > 0 && 0 < a < 1 && ΔV > 0 && β > 0 && 0 < c < 1]**

$$- \left(\left(2 (-1 + 2a) e^{\frac{1}{2}(1+2c)\beta \Delta V} \left(-c^2 \beta \Delta V \cosh\left[\frac{\beta \Delta V}{2}\right] (-1 + \cosh[c \beta \Delta V]) + \sinh\left[\frac{\beta \Delta V}{2}\right] \right. \right. \right. \\ \left. \left. \left((-1 + c) (2 + c (-2 + c \beta^2 \Delta V^2)) + 2 (-1 + c)^2 \cosh[c \beta \Delta V] + c^2 \beta \Delta V \sinh[c \beta \Delta V] \right) \right) \right) \Bigg) / \\ \left((-1 + c) c (-1 + e^{\beta \Delta V}) (-1 + e^{c \beta \Delta V})^2 \beta \Delta V \right)$$

jtot = FullSimplify[j1 + jc, Assumptions → L > 0 && 0 < a < 1 && ΔV > 0 && β > 0 && 0 < c < 1]

$$\frac{1}{8(-1+c)} \left((-1+2a) \operatorname{Csch}\left[\frac{c\beta\Delta V}{2}\right]^2 \left(\operatorname{Csch}\left[\frac{\beta\Delta V}{2}\right]^2 (-(-1+c)\beta\Delta V(-1-c+c\cosh[\beta\Delta V]+\cosh[c\beta\Delta V])) + (1+c)(-1+\cosh[c\beta\Delta V])\sinh[\beta\Delta V] \right) - 2(1+c)\sinh[c\beta\Delta V] \right)$$

Limit[j1, c → 0]

$$-\frac{(-1+2a)(-4-\beta\Delta V+e^{2\beta\Delta V}(-4+\beta\Delta V)+2e^{\beta\Delta V}(4+\beta^2\Delta V^2))}{2(-1+e^{\beta\Delta V})^2\beta\Delta V}$$

Limit[jc, c → 0]

$$0$$

Series[j1, {c, 1, 2}]

$$\begin{aligned} & \frac{1}{2(-1+e^{\beta\Delta V})^3\beta\Delta V} \\ & e^{\beta\Delta V} \left(-4+8a+4e^{\beta\Delta V}-8ae^{\beta\Delta V}+2e^{\frac{(1-2a)\beta\Delta V}{-1+a}+\frac{a\beta\Delta V}{-1+a}}-4ae^{\frac{(1-2a)\beta\Delta V}{-1+a}+\frac{a\beta\Delta V}{-1+a}}-2e^{\beta\Delta V+\frac{(1-2a)\beta\Delta V}{-1+a}+\frac{a\beta\Delta V}{-1+a}}+ \right. \\ & 4ae^{\beta\Delta V+\frac{(1-2a)\beta\Delta V}{-1+a}+\frac{a\beta\Delta V}{-1+a}}+2e^{\frac{(1-2a)\beta\Delta V}{-1+a}+\frac{(-2+3a)\beta\Delta V}{-1+a}}-4ae^{\frac{(1-2a)\beta\Delta V}{-1+a}+\frac{(-2+3a)\beta\Delta V}{-1+a}}- \\ & 2e^{\beta\Delta V+\frac{(1-2a)\beta\Delta V}{-1+a}+\frac{(-2+3a)\beta\Delta V}{-1+a}}+4ae^{\beta\Delta V+\frac{(1-2a)\beta\Delta V}{-1+a}+\frac{(-2+3a)\beta\Delta V}{-1+a}}+4\beta\Delta V-8a\beta\Delta V+ \\ & 4e^{\beta\Delta V}\beta\Delta V-8ae^{\beta\Delta V}\beta\Delta V-4e^{\beta\Delta V+\frac{(1-2a)\beta\Delta V}{-1+a}+\frac{a\beta\Delta V}{-1+a}}\beta\Delta V+8ae^{\beta\Delta V+\frac{(1-2a)\beta\Delta V}{-1+a}+\frac{a\beta\Delta V}{-1+a}}\beta\Delta V- \\ & 4e^{\frac{(1-2a)\beta\Delta V}{-1+a}+\frac{(-2+3a)\beta\Delta V}{-1+a}}\beta\Delta V+8ae^{\frac{(1-2a)\beta\Delta V}{-1+a}+\frac{(-2+3a)\beta\Delta V}{-1+a}}\beta\Delta V-2a\beta^2\Delta V^2-2e^{\beta\Delta V}\beta^2\Delta V^2+ \\ & 2ae^{\beta\Delta V}\beta^2\Delta V^2+2ae^{\beta\Delta V+\frac{(1-2a)\beta\Delta V}{-1+a}+\frac{a\beta\Delta V}{-1+a}}\beta^2\Delta V^2+2e^{\frac{(1-2a)\beta\Delta V}{-1+a}+\frac{(-2+3a)\beta\Delta V}{-1+a}}\beta^2\Delta V^2- \\ & 2ae^{\frac{(1-2a)\beta\Delta V}{-1+a}+\frac{(-2+3a)\beta\Delta V}{-1+a}}\beta^2\Delta V^2+\beta^3\Delta V^3-2a\beta^3\Delta V^3+e^{\beta\Delta V}\beta^3\Delta V^3-2ae^{\beta\Delta V}\beta^3\Delta V^3 \Big) (c-1) + \\ & \frac{1}{(-1+e^{\beta\Delta V})\beta\Delta V} \left(\left(-e^{\frac{a\beta\Delta V}{-1+a}}(-1+2a+a\beta\Delta V)+e^{\frac{(-1+2a)\beta\Delta V}{-1+a}}(-1+2a+a\beta\Delta V)- \right. \right. \\ & \frac{(-1+2a)e^{\frac{a\beta\Delta V}{-1+a}}\beta\Delta V(-2+4a+a\beta\Delta V)}{-1+a} + \\ & \frac{(-2+3a)e^{\frac{(-2+3a)\beta\Delta V}{-1+a}}\beta\Delta V(2-4a-\beta\Delta V+a\beta\Delta V)}{-1+a} - e^{\frac{(-1+2a)\beta\Delta V}{-1+a}}(1-2a-\beta\Delta V+a\beta\Delta V) + \\ & e^{\frac{(-2+3a)\beta\Delta V}{-1+a}}(1-2a-\beta\Delta V+a\beta\Delta V) - \frac{(-1+2a)^2e^{\frac{(-1+2a)\beta\Delta V}{-1+a}}\beta^2\Delta V^2(-\beta\Delta V+2a\beta\Delta V)}{2(-1+a)^2} + \\ & \left. \left. \frac{(-2+3a)^2e^{\frac{(-1+2a)\beta\Delta V}{-1+a}}\beta^2\Delta V^2(-\beta\Delta V+2a\beta\Delta V)}{2(-1+a)^2} - \frac{1}{-1+a}(-1+2a)e^{\frac{(-1+2a)\beta\Delta V}{-1+a}}\beta\Delta V \right) \right) \end{aligned}$$

$$\begin{aligned}
& (2 - 4a - 2\beta\Delta V + 3a\beta\Delta V) + \frac{1}{-1+a} (-2+3a) e^{\frac{(-1+2a)\beta\Delta V}{-1+a}} \beta\Delta V (-2+4a-\beta\Delta V+3a\beta\Delta V) \Bigg) \\
& \left(-\frac{e^{\beta\Delta V + \frac{(1-2a)\beta\Delta V}{-1+a}} \beta\Delta V}{(-1+e^{\beta\Delta V})^2} + \frac{-e^{\frac{(1-2a)\beta\Delta V}{-1+a}} + \frac{(2-3a)e^{\frac{(1-2a)\beta\Delta V}{-1+a}} \beta\Delta V}{-1+a}}{1-e^{-\beta\Delta V}} \right) + \frac{1}{1-e^{-\beta\Delta V}} e^{\frac{(1-2a)\beta\Delta V}{-1+a}} \\
& \left(-\frac{(-1+2a)e^{\frac{a\beta\Delta V}{-1+a}} \beta\Delta V (-1+2a+a\beta\Delta V)}{-1+a} + \frac{(-2+3a)e^{\frac{(-1+2a)\beta\Delta V}{-1+a}} \beta\Delta V (-1+2a+a\beta\Delta V)}{-1+a} - \right. \\
& \frac{1}{2} e^{\frac{a\beta\Delta V}{-1+a}} \left(2\beta\Delta V + \frac{\beta\Delta V}{-1+a} \right)^2 (-2+4a+a\beta\Delta V) - \frac{1}{-1+a} (-1+2a) e^{\frac{(-1+2a)\beta\Delta V}{-1+a}} \beta \\
& \Delta V (1-2a-\beta\Delta V+a\beta\Delta V) - \frac{(-1+2a)^3 e^{\frac{(-1+2a)\beta\Delta V}{-1+a}} \beta^3 \Delta V^3 (-\beta\Delta V+2a\beta\Delta V)}{6(-1+a)^3} + \\
& \frac{(-2+3a)^3 e^{\frac{(-1+2a)\beta\Delta V}{-1+a}} \beta^3 \Delta V^3 (-\beta\Delta V+2a\beta\Delta V)}{6(-1+a)^3} - \frac{1}{2(-1+a)^2} \\
& (-1+2a)^2 e^{\frac{(-1+2a)\beta\Delta V}{-1+a}} \beta^2 \Delta V^2 (2-4a-2\beta\Delta V+3a\beta\Delta V) + \frac{1}{2(-1+a)^2} (-2+3a)^2 \\
& e^{\frac{(-1+2a)\beta\Delta V}{-1+a}} \beta^2 \Delta V^2 (-2+4a-\beta\Delta V+3a\beta\Delta V) + \frac{1}{2(-1+a)^2} (-2+3a) e^{\frac{(-2+3a)\beta\Delta V}{-1+a}} \beta\Delta V \\
& \left. (-2+6a-4a^2-2\beta\Delta V+10a\beta\Delta V-10a^2\beta\Delta V+2\beta^2\Delta V^2-5a\beta^2\Delta V^2+3a^2\beta^2\Delta V^2) \right) + \\
& \left(-e^{\frac{a\beta\Delta V}{-1+a}} (-2+4a+a\beta\Delta V) + e^{\frac{(-2+3a)\beta\Delta V}{-1+a}} (2-4a-\beta\Delta V+a\beta\Delta V) - \right. \\
& \frac{(-1+2a)e^{\frac{(-1+2a)\beta\Delta V}{-1+a}} \beta\Delta V (-\beta\Delta V+2a\beta\Delta V)}{-1+a} + \\
& \frac{(-2+3a)e^{\frac{(-1+2a)\beta\Delta V}{-1+a}} \beta\Delta V (-\beta\Delta V+2a\beta\Delta V)}{-1+a} - \\
& \left. e^{\frac{(-1+2a)\beta\Delta V}{-1+a}} (2-4a-2\beta\Delta V+3a\beta\Delta V) + e^{\frac{(-1+2a)\beta\Delta V}{-1+a}} (-2+4a-\beta\Delta V+3a\beta\Delta V) \right) \\
& \left(\frac{e^{\beta\Delta V + \frac{(1-2a)\beta\Delta V}{-1+a}} (1+e^{\beta\Delta V}) \beta^2 \Delta V^2}{2(-1+e^{\beta\Delta V})^3} - \frac{e^{\beta\Delta V} \beta\Delta V \left(-e^{\frac{(1-2a)\beta\Delta V}{-1+a}} + \frac{(2-3a)e^{\frac{(1-2a)\beta\Delta V}{-1+a}} \beta\Delta V}{-1+a} \right)}{(-1+e^{\beta\Delta V})^2} + \frac{1}{1-e^{-\beta\Delta V}} \right)
\end{aligned}$$

$$\left(e^{\frac{(1-2a)\beta\Delta V}{-1+a}} - \frac{(2-3a)e^{\frac{(1-2a)\beta\Delta V}{-1+a}}\beta\Delta V}{-1+a} + \frac{(2-3a)^2e^{\frac{(1-2a)\beta\Delta V}{-1+a}}\beta^2\Delta V^2}{2(-1+a)^2} \right) \Bigg) (c-1)^2 + O[c-1]^3$$

Series[jc, {c, 1, 2}]

$$\begin{aligned} & - \frac{1}{(-1 + e^{\beta\Delta V})^3 \beta \Delta V} 2 \left((-1 + 2a) e^{\frac{3\beta\Delta V}{2}} \right. \\ & \quad \left(\beta \Delta V \cosh\left[\frac{\beta\Delta V}{2}\right] \left(1 - \cosh[\beta\Delta V] - \frac{1}{2}\beta^2\Delta V^2 \cosh[\beta\Delta V] - 2\beta\Delta V \sinh[\beta\Delta V] \right) + \right. \\ & \quad \sinh\left[\frac{\beta\Delta V}{2}\right] \left(-2 + 2\beta^2\Delta V^2 + 2\cosh[\beta\Delta V] + 2\beta^2\Delta V^2 \cosh[\beta\Delta V] + \right. \\ & \quad \left. \beta\Delta V \sinh[\beta\Delta V] + \frac{1}{2}\beta^3\Delta V^3 \sinh[\beta\Delta V] \right) \Bigg) (c-1) - \\ & \frac{1}{(-1 + e^{\beta\Delta V}) \beta \Delta V} 2 \left((-1 + 2a) \left(\left(-\frac{2e^{\frac{5\beta\Delta V}{2}}\beta\Delta V}{(-1 + e^{\beta\Delta V})^3} + \frac{-e^{\frac{3\beta\Delta V}{2}} + e^{\frac{3\beta\Delta V}{2}}\beta\Delta V}{(-1 + e^{\beta\Delta V})^2} \right) \right. \right. \\ & \quad \left(\beta \Delta V \cosh\left[\frac{\beta\Delta V}{2}\right] \left(1 - \cosh[\beta\Delta V] - \frac{1}{2}\beta^2\Delta V^2 \cosh[\beta\Delta V] - 2\beta\Delta V \sinh[\beta\Delta V] \right) + \right. \\ & \quad \sinh\left[\frac{\beta\Delta V}{2}\right] \left(-2 + 2\beta^2\Delta V^2 + 2\cosh[\beta\Delta V] + 2\beta^2\Delta V^2 \cosh[\beta\Delta V] + \right. \\ & \quad \left. \beta\Delta V \sinh[\beta\Delta V] + \frac{1}{2}\beta^3\Delta V^3 \sinh[\beta\Delta V] \right) \Bigg) + \frac{1}{(-1 + e^{\beta\Delta V})^2} \\ & e^{\frac{3\beta\Delta V}{2}} \left(\beta \Delta V \cosh\left[\frac{\beta\Delta V}{2}\right] \left(-\beta^2\Delta V^2 \cosh[\beta\Delta V] - \beta\Delta V \sinh[\beta\Delta V] - \frac{1}{6}\beta^3\Delta V^3 \sinh[\beta\Delta V] \right) + \right. \\ & \quad \sinh\left[\frac{\beta\Delta V}{2}\right] \left(\beta^2\Delta V^2 + \beta^2\Delta V^2 \cosh[\beta\Delta V] + \frac{1}{6}\beta^4\Delta V^4 \cosh[\beta\Delta V] + \right. \\ & \quad \left. \left. 2\beta\Delta V \sinh[\beta\Delta V] + \beta^3\Delta V^3 \sinh[\beta\Delta V] \right) \Bigg) \Bigg) (c-1)^2 + O[c-1]^3 \end{aligned}$$

$$\begin{aligned}
j11 = & \frac{1}{2 \left(-1 + e^{\beta \Delta V}\right)^3 \beta \Delta V} e^{\beta \Delta V} \\
& \left(-4 + 8a + 4e^{\beta \Delta V} - 8ae^{\beta \Delta V} + 2e^{\frac{(1-2a)\beta \Delta V}{-1+a} + \frac{a\beta \Delta V}{-1+a}} - 4ae^{\frac{(1-2a)\beta \Delta V}{-1+a} + \frac{a\beta \Delta V}{-1+a}} - 2e^{\beta \Delta V + \frac{(1-2a)\beta \Delta V}{-1+a} + \frac{a\beta \Delta V}{-1+a}} + \right. \\
& 4ae^{\beta \Delta V + \frac{(1-2a)\beta \Delta V}{-1+a} + \frac{a\beta \Delta V}{-1+a}} + 2e^{\frac{(1-2a)\beta \Delta V}{-1+a} + \frac{(-2+3a)\beta \Delta V}{-1+a}} - 4ae^{\frac{(1-2a)\beta \Delta V}{-1+a} + \frac{(-2+3a)\beta \Delta V}{-1+a}} - 2e^{\beta \Delta V + \frac{(1-2a)\beta \Delta V}{-1+a} + \frac{(-2+3a)\beta \Delta V}{-1+a}} + \\
& 4ae^{\beta \Delta V + \frac{(1-2a)\beta \Delta V}{-1+a} + \frac{(-2+3a)\beta \Delta V}{-1+a}} + 4\beta \Delta V - 8a\beta \Delta V + 4e^{\beta \Delta V} \beta \Delta V - 8ae^{\beta \Delta V} \beta \Delta V - \\
& 4e^{\beta \Delta V + \frac{(1-2a)\beta \Delta V}{-1+a} + \frac{a\beta \Delta V}{-1+a}} \beta \Delta V + 8ae^{\beta \Delta V + \frac{(1-2a)\beta \Delta V}{-1+a} + \frac{a\beta \Delta V}{-1+a}} \beta \Delta V - 4e^{\frac{(1-2a)\beta \Delta V}{-1+a} + \frac{(-2+3a)\beta \Delta V}{-1+a}} \beta \Delta V + \\
& 8ae^{\frac{(1-2a)\beta \Delta V}{-1+a} + \frac{(-2+3a)\beta \Delta V}{-1+a}} \beta \Delta V - 2a\beta^2 \Delta V^2 - 2e^{\beta \Delta V} \beta^2 \Delta V^2 + 2ae^{\beta \Delta V} \beta^2 \Delta V^2 + \\
& 2ae^{\beta \Delta V + \frac{(1-2a)\beta \Delta V}{-1+a} + \frac{a\beta \Delta V}{-1+a}} \beta^2 \Delta V^2 + 2e^{\frac{(1-2a)\beta \Delta V}{-1+a} + \frac{(-2+3a)\beta \Delta V}{-1+a}} \beta^2 \Delta V^2 - 2ae^{\frac{(1-2a)\beta \Delta V}{-1+a} + \frac{(-2+3a)\beta \Delta V}{-1+a}} \beta^2 \Delta V^2 + \\
& \left. \beta^3 \Delta V^3 - 2a\beta^3 \Delta V^3 + e^{\beta \Delta V} \beta^3 \Delta V^3 - 2ae^{\beta \Delta V} \beta^3 \Delta V^3 \right) (c-1) \\
\\
& \frac{1}{2 \left(-1 + e^{\beta \Delta V}\right)^3 \beta \Delta V} \\
& (-1+c) e^{\beta \Delta V} \left(-4 + 8a + 4e^{\beta \Delta V} - 8ae^{\beta \Delta V} + 2e^{\frac{(1-2a)\beta \Delta V}{-1+a} + \frac{a\beta \Delta V}{-1+a}} - 4ae^{\frac{(1-2a)\beta \Delta V}{-1+a} + \frac{a\beta \Delta V}{-1+a}} - 2e^{\beta \Delta V + \frac{(1-2a)\beta \Delta V}{-1+a} + \frac{a\beta \Delta V}{-1+a}} + \right. \\
& 4ae^{\beta \Delta V + \frac{(1-2a)\beta \Delta V}{-1+a} + \frac{a\beta \Delta V}{-1+a}} + 2e^{\frac{(1-2a)\beta \Delta V}{-1+a} + \frac{(-2+3a)\beta \Delta V}{-1+a}} - 4ae^{\frac{(1-2a)\beta \Delta V}{-1+a} + \frac{(-2+3a)\beta \Delta V}{-1+a}} - \\
& 2e^{\beta \Delta V + \frac{(1-2a)\beta \Delta V}{-1+a} + \frac{(-2+3a)\beta \Delta V}{-1+a}} + 4ae^{\beta \Delta V + \frac{(1-2a)\beta \Delta V}{-1+a} + \frac{(-2+3a)\beta \Delta V}{-1+a}} + 4\beta \Delta V - 8a\beta \Delta V + \\
& 4e^{\beta \Delta V} \beta \Delta V - 8ae^{\beta \Delta V} \beta \Delta V - 4e^{\beta \Delta V + \frac{(1-2a)\beta \Delta V}{-1+a} + \frac{a\beta \Delta V}{-1+a}} \beta \Delta V + 8ae^{\beta \Delta V + \frac{(1-2a)\beta \Delta V}{-1+a} + \frac{a\beta \Delta V}{-1+a}} \beta \Delta V - \\
& 4e^{\frac{(1-2a)\beta \Delta V}{-1+a} + \frac{(-2+3a)\beta \Delta V}{-1+a}} \beta \Delta V + 8ae^{\frac{(1-2a)\beta \Delta V}{-1+a} + \frac{(-2+3a)\beta \Delta V}{-1+a}} \beta \Delta V - 2a\beta^2 \Delta V^2 - 2e^{\beta \Delta V} \beta^2 \Delta V^2 + \\
& 2ae^{\beta \Delta V} \beta^2 \Delta V^2 + 2ae^{\beta \Delta V + \frac{(1-2a)\beta \Delta V}{-1+a} + \frac{a\beta \Delta V}{-1+a}} \beta^2 \Delta V^2 + 2e^{\frac{(1-2a)\beta \Delta V}{-1+a} + \frac{(-2+3a)\beta \Delta V}{-1+a}} \beta^2 \Delta V^2 - \\
& \left. 2ae^{\frac{(1-2a)\beta \Delta V}{-1+a} + \frac{(-2+3a)\beta \Delta V}{-1+a}} \beta^2 \Delta V^2 + \beta^3 \Delta V^3 - 2a\beta^3 \Delta V^3 + e^{\beta \Delta V} \beta^3 \Delta V^3 - 2ae^{\beta \Delta V} \beta^3 \Delta V^3 \right) \\
\\
jcl = & -\frac{1}{\left(-1 + e^{\beta \Delta V}\right)^3 \beta \Delta V} 2 \\
& \left((-1+2a) e^{\frac{3\beta \Delta V}{2}} \left(\beta \Delta V \cosh\left[\frac{\beta \Delta V}{2}\right] \left(1 - \cosh[\beta \Delta V] - \frac{1}{2} \beta^2 \Delta V^2 \cosh[\beta \Delta V] - 2\beta \Delta V \sinh[\beta \Delta V] \right) + \right. \right. \\
& \sinh\left[\frac{\beta \Delta V}{2}\right] \left(-2 + 2\beta^2 \Delta V^2 + 2\cosh[\beta \Delta V] + 2\beta^2 \Delta V^2 \cosh[\beta \Delta V] + \right. \\
& \left. \left. \beta \Delta V \sinh[\beta \Delta V] + \frac{1}{2} \beta^3 \Delta V^3 \sinh[\beta \Delta V] \right) \right) \right) (c-1) \\
\\
& -\frac{1}{\left(-1 + e^{\beta \Delta V}\right)^3 \beta \Delta V} 2 (-1+2a) (-1+c) e^{\frac{3\beta \Delta V}{2}} \\
& \left(\beta \Delta V \cosh\left[\frac{\beta \Delta V}{2}\right] \left(1 - \cosh[\beta \Delta V] - \frac{1}{2} \beta^2 \Delta V^2 \cosh[\beta \Delta V] - 2\beta \Delta V \sinh[\beta \Delta V] \right) + \right. \\
& \sinh\left[\frac{\beta \Delta V}{2}\right] \left(-2 + 2\beta^2 \Delta V^2 + 2\cosh[\beta \Delta V] + \right. \\
& \left. \left. 2\beta^2 \Delta V^2 \cosh[\beta \Delta V] + \beta \Delta V \sinh[\beta \Delta V] + \frac{1}{2} \beta^3 \Delta V^3 \sinh[\beta \Delta V] \right) \right)
\end{aligned}$$

Simplify[j11+jcl, Assumptions $\rightarrow L > 0 \ \&\& \ 0 < a < 1 \ \&\& \ \Delta V > 0 \ \&\& \ \beta > 0 \ \&\& \ 0 < c < 1$]

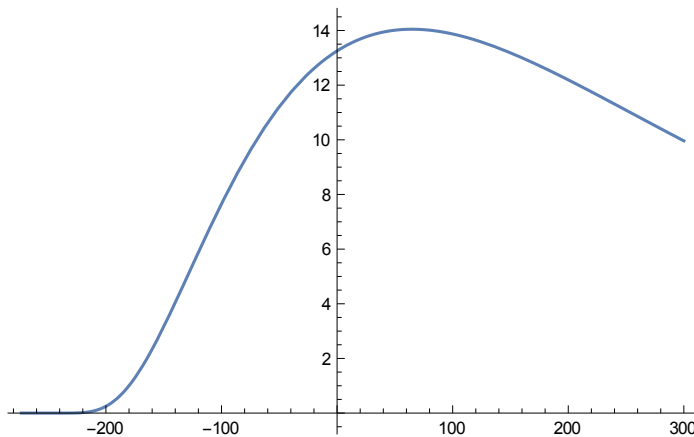
```
Series[Log[jtot], {c, 0, 3}]
```

[illegible]

$$\begin{aligned}
& \left(2 \left(6 + \beta^2 \Delta V^2 - 3 \operatorname{Csch} \left[\frac{\beta \Delta V}{2} \right]^2 + 3 \operatorname{Cosh}[\beta \Delta V] \operatorname{Csch} \left[\frac{\beta \Delta V}{2} \right]^2 - \right. \right. \\
& \quad \left. \left. 3 \beta \Delta V \operatorname{Csch} \left[\frac{\beta \Delta V}{2} \right]^2 \operatorname{Sinh}[\beta \Delta V] \right) \right. \\
& \quad \left(\left(4 \left(6 + \beta^2 \Delta V^2 - 3 \operatorname{Csch} \left[\frac{\beta \Delta V}{2} \right]^2 + 3 \operatorname{Cosh}[\beta \Delta V] \operatorname{Csch} \left[\frac{\beta \Delta V}{2} \right]^2 - 3 \beta \Delta V \operatorname{Csch} \left[\frac{\beta \Delta V}{2} \right]^2 \right. \right. \right. \\
& \quad \left. \left. \left. \operatorname{Sinh}[\beta \Delta V] \right)^2 \right) / \left(9 \left(-4 + 2 \operatorname{Csch} \left[\frac{\beta \Delta V}{2} \right]^2 + \beta^2 \Delta V^2 \operatorname{Csch} \left[\frac{\beta \Delta V}{2} \right]^2 - \right. \right. \right. \\
& \quad \left. \left. \left. 2 \operatorname{Cosh}[\beta \Delta V] \operatorname{Csch} \left[\frac{\beta \Delta V}{2} \right]^2 + \beta \Delta V \operatorname{Csch} \left[\frac{\beta \Delta V}{2} \right]^2 \operatorname{Sinh}[\beta \Delta V] \right)^2 \right) - \right. \\
& \quad \left(-24 - 6 \beta^2 \Delta V^2 + 12 \operatorname{Csch} \left[\frac{\beta \Delta V}{2} \right]^2 - \beta^2 \Delta V^2 \operatorname{Csch} \left[\frac{\beta \Delta V}{2} \right]^2 - 12 \operatorname{Cosh}[\beta \Delta V] \operatorname{Csch} \left[\frac{\beta \Delta V}{2} \right]^2 + \right. \\
& \quad \left. \left. \beta^2 \Delta V^2 \operatorname{Cosh}[\beta \Delta V] \operatorname{Csch} \left[\frac{\beta \Delta V}{2} \right]^2 + 12 \beta \Delta V \operatorname{Csch} \left[\frac{\beta \Delta V}{2} \right]^2 \operatorname{Sinh}[\beta \Delta V] \right) / \right. \\
& \quad \left(6 \left(-4 + 2 \operatorname{Csch} \left[\frac{\beta \Delta V}{2} \right]^2 + \beta^2 \Delta V^2 \operatorname{Csch} \left[\frac{\beta \Delta V}{2} \right]^2 - 2 \operatorname{Cosh}[\beta \Delta V] \operatorname{Csch} \left[\frac{\beta \Delta V}{2} \right]^2 + \right. \right. \\
& \quad \left. \left. \left. \beta \Delta V \operatorname{Csch} \left[\frac{\beta \Delta V}{2} \right]^2 \operatorname{Sinh}[\beta \Delta V] \right) \right) \right) / \right. \\
& \quad \left(3 \left(-4 + 2 \operatorname{Csch} \left[\frac{\beta \Delta V}{2} \right]^2 + \beta^2 \Delta V^2 \operatorname{Csch} \left[\frac{\beta \Delta V}{2} \right]^2 - 2 \operatorname{Cosh}[\beta \Delta V] \operatorname{Csch} \left[\frac{\beta \Delta V}{2} \right]^2 + \right. \right. \\
& \quad \left. \left. \left. \beta \Delta V \operatorname{Csch} \left[\frac{\beta \Delta V}{2} \right]^2 \operatorname{Sinh}[\beta \Delta V] \right) \right) \right) \right) c^3 + O[c]^4
\end{aligned}$$

`Plot[lu lb / (lu + lb) L jtot //.`

`{a → 1 / 4, ΔV → 40, β → 310.15 / (4.28 (T + 273.15)), L → 8, lu → 40, lb → 80, c → 0.2},`
`{T, -273.15, 300}, PlotRange → All]`



`Limit[lu lb / (lu + lb) L jtot //.`

`{a → 1 / 4, ΔV → 40, β → 1 / 4.28, L → 8, lu → 40, lb → 80}, c → 0.3]`

7.85977

Series[j1, {β, 0, 3}]

$$\frac{1}{720} \left(2 \Delta V^3 - 4 a \Delta V^3 - c \Delta V^3 + 2 a c \Delta V^3 - c^2 \Delta V^3 + 2 a c^2 \Delta V^3 \right) \beta^3 + O[\beta]^4$$

Series[jc, {β, 0, 3}]

$$-\frac{1}{720} \left((-1 + c) \left(-c \Delta V^3 + 2 a c \Delta V^3 - 2 c^2 \Delta V^3 + 4 a c^2 \Delta V^3 \right) \right) \beta^3 + O[\beta]^4$$

**fVVV = Simplify[full[Exp[β V[#]] &, V[#] Exp[-β V[#]] &],
Assumptions → L > 0 && 0 < a < 1 && ΔV > 0 && β > 0]**

$$-\frac{1}{2 \beta^4 \Delta V^3} e^{-\beta \Delta V} L^2 \left(6 + 4 \beta \Delta V + e^{2 \beta \Delta V} (6 - 2 \beta \Delta V) - e^{\beta \Delta V} (12 + 2 \beta \Delta V + \beta^3 \Delta V^3) + \right. \\ \left. 2 a (-6 - 5 \beta \Delta V - \beta^2 \Delta V^2 + e^{2 \beta \Delta V} (-6 + \beta \Delta V) + e^{\beta \Delta V} (12 + 4 \beta \Delta V + \beta^2 \Delta V^2 + \beta^3 \Delta V^3)) \right)$$

**FullSimplify[β (fVVV + Simplify[D[Log[Z[β]], β]] fVV) / (Z[β] Z[-β]),
Assumptions → L > 0 && 0 < a < 1 && ΔV > 0 && β > 0]**

$$-\frac{1}{2 (-1 + e^{\beta \Delta V})^3 \beta \Delta V} \\ (-1 + 2 a) e^{-\frac{a \beta \Delta V}{-1+a}} \left(2 e^{\frac{a \beta \Delta V}{-1+a}} - 2 e^{\frac{(-3+4 a) \beta \Delta V}{-1+a}} + e^{\left(2+\frac{1}{-1+a}\right) \beta \Delta V} (-6 + \beta^3 \Delta V^3) + e^{\left(3+\frac{1}{-1+a}\right) \beta \Delta V} (6 + \beta^3 \Delta V^3) \right)$$

FullSimplify[% / (a - 1 / 2) (1 - Exp[-β ΔV])^3,

Assumptions → L > 0 && 0 < a < 1 && ΔV > 0 && β > 0]

$$\frac{1}{\beta \Delta V} e^{-\left(4+\frac{1}{-1+a}\right) \beta \Delta V} \left(2 e^{\left(4+\frac{1}{-1+a}\right) \beta \Delta V} - 2 e^{\frac{a \beta \Delta V}{-1+a}} + e^{\left(2+\frac{1}{-1+a}\right) \beta \Delta V} (6 - \beta^3 \Delta V^3) - e^{\left(3+\frac{1}{-1+a}\right) \beta \Delta V} (6 + \beta^3 \Delta V^3) \right)$$

Expand[%]

$$\frac{2}{\beta \Delta V} + \frac{6 e^{\left(2+\frac{1}{-1+a}\right) \beta \Delta V} \left(4+\frac{1}{-1+a}\right) \beta \Delta V}{\beta \Delta V} - \frac{6 e^{\left(3+\frac{1}{-1+a}\right) \beta \Delta V} \left(4+\frac{1}{-1+a}\right) \beta \Delta V}{\beta \Delta V} - \\ \frac{2 e^{-\left(4+\frac{1}{-1+a}\right) \beta \Delta V} e^{\frac{a \beta \Delta V}{-1+a}}}{\beta \Delta V} - e^{\left(2+\frac{1}{-1+a}\right) \beta \Delta V} \left(4+\frac{1}{-1+a}\right) \beta \Delta V \beta^2 \Delta V^2 - e^{\left(3+\frac{1}{-1+a}\right) \beta \Delta V} \left(4+\frac{1}{-1+a}\right) \beta \Delta V \beta^2 \Delta V^2$$

Map[Simplify[#] &, %]

$$\frac{2}{\beta \Delta V} - \frac{2 e^{-3 \beta \Delta V}}{\beta \Delta V} + \frac{6 e^{-2 \beta \Delta V}}{\beta \Delta V} - \frac{6 e^{-\beta \Delta V}}{\beta \Delta V} - e^{-2 \beta \Delta V} \beta^2 \Delta V^2 - e^{-\beta \Delta V} \beta^2 \Delta V^2$$

**FullSimplify[β (fVVV + Simplify[D[Log[Z[β]], β]] fVV) / (Z[β] Z[-β]) -
(a - 1 / 2) (2 / (β ΔV) - (β ΔV)^2 Exp[-β ΔV] (1 + Exp[-β ΔV]) (1 - Exp[-β ΔV])^-3),
Assumptions → L > 0 && 0 < a < 1 && ΔV > 0 && β > 0]**

0

`Series[(a - 1/2) (2/(β ΔV) - (β ΔV)2/4 Cosh[β ΔV/2] (Sinh[β ΔV/2])-3), {β, 0, 4}]`

$$\left(-\frac{\Delta V^3}{240} + \frac{a \Delta V^3}{120}\right) \beta^3 + O[\beta]^5$$

`NSolve[(D[jtot, β] == 0) /. {ΔV → 40, a → 1/4, c → 3/10}, β]`

`ReplaceAll::reps: {{ΔV → 40, a → 1/4, c → 3/10} == 0}` is neither a list of

replacement rules nor a valid dispatch table, and so cannot be used for replacing. >>

`ReplaceAll::reps: {(ΔV → 40) == 0 && (a → 1/4) == 0 && (c → 3/10) == 0}` is neither a list

of replacement rules nor a valid dispatch table, and so cannot be used for replacing. >>

`NSolve::nsmet: This system cannot be solved with the methods available to NSolve. >>`

$$\begin{aligned} & \text{NSolve}\left[-\frac{1}{8(-1+c)}(-1+2a)c\Delta V\coth\left[\frac{c\beta\Delta V}{2}\right]\text{csch}\left[\frac{c\beta\Delta V}{2}\right]^2\right. \\ & \quad \left(\text{csch}\left[\frac{\beta\Delta V}{2}\right]^2(-(-1+c)\beta\Delta V(-1-c+c\cosh[\beta\Delta V]+\cosh[c\beta\Delta V]))+\right. \\ & \quad \left.(1+c)(-1+\cosh[c\beta\Delta V])\sinh[\beta\Delta V]-2(1+c)\sinh[c\beta\Delta V]\right)+ \\ & \quad \frac{1}{8(-1+c)}(-1+2a)\text{csch}\left[\frac{c\beta\Delta V}{2}\right]^2\left(-2c(1+c)\Delta V\cosh[c\beta\Delta V]-\right. \\ & \quad \Delta V\coth\left[\frac{\beta\Delta V}{2}\right]\text{csch}\left[\frac{\beta\Delta V}{2}\right]^2(-(-1+c)\beta\Delta V(-1-c+c\cosh[\beta\Delta V]+\cosh[c\beta\Delta V]))+ \\ & \quad (1+c)(-1+\cosh[c\beta\Delta V])\sinh[\beta\Delta V]+ \\ & \quad \left.\text{csch}\left[\frac{\beta\Delta V}{2}\right]^2((1+c)\Delta V\cosh[\beta\Delta V](-1+\cosh[c\beta\Delta V])-(1+c)\Delta V(-1-c+ \right. \\ & \quad \left. c\cosh[\beta\Delta V]+\cosh[c\beta\Delta V])+c(1+c)\Delta V\sinh[\beta\Delta V]\sinh[c\beta\Delta V]-(-1+c)\beta\right. \\ & \quad \left.\Delta V(c\Delta V\sinh[\beta\Delta V]+c\Delta V\sinh[c\beta\Delta V]))\right)/.\left\{\Delta V\rightarrow 40, a\rightarrow \frac{1}{4}, c\rightarrow \frac{3}{10}\right\}=0, \beta\Big] \end{aligned}$$