Numerical Methods in Chemistry

Solutions to Exercises 1

Problem 1

(a)

$$\mathcal{L}\left\{e^{kt}\right\} = \int_0^\infty e^{kt} e^{-st}\,\mathrm{d}t = \int_0^\infty e^{(k-s)t}\,\mathrm{d}t \overset{\mathrm{Re}(s)>\mathrm{Re}(k)}{=} \left[\frac{1}{k-s}\,e^{(k-s)t}\right]_0^\infty = \frac{1}{s-k}.$$

(b)

$$\mathcal{L}\left\{t^2\right\} = \int_0^\infty t^2 e^{-st}\,\mathrm{d}t \overset{\text{by parts}}{=} \left[-\frac{t^2}{s}\,e^{-st}\right]_0^\infty + \int_0^\infty \frac{2t}{s}\,e^{-st}\,\mathrm{d}t \overset{\mathrm{Re}(s)>0}{=} \frac{2}{s}\int_0^\infty t\,e^{-st}\,\mathrm{d}t \overset{\text{by parts}}{=}$$

$$= \frac{2}{s}\left\{\left[-\frac{t}{s}\,e^{-st}\right]_0^\infty + \int_0^\infty \frac{e^{-st}}{s}\,\mathrm{d}t\right\} \overset{\mathrm{Re}(s)>0}{=} \frac{2}{s^2}\left[-\frac{e^{-st}}{s}\right]_0^\infty = \frac{2}{s^3}.$$

(c)

$$\mathcal{L}\left\{\cosh t\right\} = \mathcal{L}\left\{\frac{e^t+e^{-t}}{2}\right\} \overset{\text{linearity}}{=} \frac{1}{2}\left[\underbrace{\int_0^\infty e^t\,e^{-st}\,\mathrm{d}t}_{\mathrm{Re}(s)>1} + \underbrace{\int_0^\infty e^{-t}\,e^{-st}\,\mathrm{d}t}_{\mathrm{Re}(s)>-1}\right] =$$

$$\overset{\text{part (a)}}{=} \frac{1}{2}\left[\frac{1}{s-1}+\frac{1}{s+1}\right] = \frac{1}{2}\,\frac{(s+1)+(s-1)}{(s-1)(s+1)} = \frac{s}{s^2-1}.$$

Problem 2

(a) One can use the 1^{st} shift theorem:

$$\mathcal{L}\left\{e^{-bt}f(t)\right\} = F(s+b).$$

In our case, we identify

$$b = 3, \quad f(t) = t^2, \quad F(s) = \mathcal{L}\left\{t^2\right\} = \frac{2}{s^3}.$$

Application of the 1st shift theorem yields:

$$\mathcal{L}\left\{t^2\, e^{-3t}\right\} \overset{1^{\text{st}}\text{shift theorem}}{=} \frac{2}{(s+3)^3}.$$

(b)

$$\mathcal{L}\left\{4t + 6e^{4t}\right\} \overset{\text{linearity}}{=} 4\,\mathcal{L}\left\{t\right\} + 6\,\mathcal{L}\left\{e^{4t}\right\} \overset{\text{E.g. 3, pr. 1(a)}}{=} \frac{4}{s^2} + \frac{6}{s-4}.$$

(c) One can the 1st shift theorem with

$$b = 4, \quad f(t) = \sin(5t), \quad F(s) = \mathcal{L}\left\{\sin(5t)\right\} \overset{\text{E.g. 5}}{=} \frac{5}{s^2+25}.$$

Application of the 1st shift theorem yields:

$$\mathcal{L}\left\{e^{-4t}\sin(5t)\right\} \overset{1^{\text{st}}\text{shift theorem}}{=} \frac{5}{(s+4)^2+25} = \frac{5}{s^2+8s+41}.$$

Problem 3

Recall property (2) from the lecture:

$$\mathcal{L}\left\{t^n f(t)\right\} = (-1)^n \frac{\mathrm{d}^n}{\mathrm{d}s^n} F(s).$$

(a) We need to use property (2) with

$$n = 1, \quad f(t) = e^{2t}, \quad F(s) = \mathcal{L}\left\{e^{2t}\right\} \overset{\text{pr. 1(a)}}{=} \frac{1}{s-2}, \quad \frac{\mathrm{d}F(s)}{\mathrm{d}s} = -\frac{1}{(s-2)^2}.$$

Thus we obtain:

$$\mathcal{L}\left\{t\, e^{2t}\right\} = \frac{1}{(s-2)^2}.$$

(b) We use property (2) with

$$n = 1, \quad f(t) = \cos t, \quad F(s) = \mathcal{L}\left\{\cos t\right\} = \frac{s}{s^2+1}, \quad \frac{\mathrm{d}F(s)}{\mathrm{d}s} = \frac{s^2+1-2s^2}{(s^2+1)^2} = \frac{1-s^2}{(s^2+1)^2}.$$

Thus we obtain:

$$\mathcal{L}\left\{t\, \cos t\right\} = \frac{s^2-1}{(s^2+1)^2}.$$

(c) We use property (2) with

$$n = 2, \quad f(t) = \cos t, \quad F(s) = \mathcal{L}\{\cos t\} = \frac{s}{s^2+1},$$

$$\frac{\mathrm{d}^2 F(s)}{\mathrm{d}s^2} \overset{\text{pr. 2(b)}}{=} \frac{\mathrm{d}}{\mathrm{d}s}\left[\frac{1-s^2}{(s^2+1)^2}\right] = \frac{-2s(s^2+1)^2 - (1-s^2)\,2(s^2+1)2s}{(s^2+1)^4} = \frac{2s^3-6s}{(s^2+1)^3}.$$

Thus we obtain:

$$\mathcal{L}\left\{t^2 \cos t\right\} = \frac{2s^3-6s}{(s^2+1)^3}.$$

Problem 4

The derivative property of the Laplace Transform is (e.g. 6 in the lecture):

$$\mathcal{L}\{f'(t)\} = sF(s) - f(0).$$

In our problem we have

$$f'(t) = -a\sin(at), \quad F(s) = \mathcal{L}\{\cos(at)\} = \frac{s}{s^2+a^2}, \quad f(0) = 1.$$

We get

$$\mathcal{L}\{-a\sin(at)\} = s\,\frac{s}{s^2+a^2} - 1,$$

$$\mathcal{L}\{\sin(at)\} = -\frac{1}{a}\,\frac{s^2-(s^2+a^2)}{s^2+a^2} = \frac{a}{s^2+a^2}.$$

Problem 5

To prove the change of scale result

$$\mathcal{L}\{f(at)\} = \frac{1}{a}\,F\left(\frac{s}{a}\right),$$

one can start from

$$\mathcal{L}\{f(at)\} = \int_0^\infty f(at)\,e^{-st}\,\mathrm{d}t,$$

and use the change of variable $u = at$, which implies

$$t = \frac{u}{a} \quad \text{and} \quad \frac{\mathrm{d}u}{\mathrm{d}t} = a \Longrightarrow \mathrm{d}t = \frac{\mathrm{d}u}{a}.$$

Therefore

$$\mathcal{L}\left\{f(at)\right\} = \int_0^\infty f(u)\, e^{-s\frac{u}{a}}\, \frac{\mathrm{d}u}{a} = \frac{1}{a}\int_0^\infty f(u)\, e^{-\frac{s}{a}u}\,\mathrm{d}u = \frac{1}{a}\, F\left(\frac{s}{a}\right).$$

(We observed that the last integral is a Laplace Transform in the variable s/a).

Now to compute $\mathcal{L}\{t\cos(6t)\}$, start from $\mathcal{L}\{6t\cos(6t)\}$ and use the change of scale for $f(t) = t\cos t$ with $a = 6$:

$$\mathcal{L}\left\{6t\cos(6t)\right\} = \mathcal{L}\left\{f(at)\right\} = \frac{1}{a}\, F\left(\frac{s}{a}\right) = \frac{1}{6}\, F\left(\frac{s}{6}\right) \overset{\text{pr. 3(b)}}{=} \frac{1}{6}\, \frac{\left(\frac{s}{6}\right)^2 - 1}{\left(\left(\frac{s}{6}\right)^2 + 1\right)^2},$$

where we used the following result from Problem 3(b):

$$F(s) = \mathcal{L}\left\{f(t)\right\} = \mathcal{L}\left\{t\cos t\right\} = \frac{s^2 - 1}{(s^2+1)^2}.$$

Hence

$$\mathcal{L}\left\{t\cos(6t)\right\} = \left(\frac{1}{6}\right)^2 F\left(\frac{s}{6}\right) = \left(\frac{1}{6}\right)^2 \frac{\left(\frac{s}{6}\right)^2 - 1}{\left(\left(\frac{s}{6}\right)^2 + 1\right)^2} = \frac{s^2 - 36}{(s^2+36)^2}.$$