## Integration III <br> Integration by parts, by substitution, with power series, and using published tables



## Answers to additional problems

21.1 We insert values with $x=3$ yields,
so

$$
\begin{aligned}
& \quad \frac{(3)^{1}}{1}+\frac{(3)^{2}}{1 \times 2}+\frac{(3)^{3}}{1 \times 2 \times 3}+\frac{(3)^{4}}{1 \times 2 \times 3 \times 4}+\ldots \frac{(3)^{9}}{1 \times 2 \times 3 \times 4 \times 5 \times 6 \times 7 \times 8 \times 9}+\ldots \\
& \text { so } \quad \mathrm{e}^{3}=1+3+\frac{9}{2}+\frac{27}{6}+\frac{81}{24}+\frac{243}{120}+\frac{729}{720}+\frac{2187}{5040}+\frac{6561}{40,320}+\frac{19683}{362,80}+\ldots \\
& \mathrm{e}^{3}=1+3+4.5+4.5+3.375+2.025+1.013+0.434+0.163+0.0542+\ldots \\
& \text { and } \quad \mathrm{e}^{3}=20.064 \text { (to } 3 \text { d.p.). }
\end{aligned}
$$

Notice how fast the terms rapidly decrease in size. This decrease enables the series to converge quickly. The answer on a pocket calculator is 20.086 so, with 10 terms, there is an error of only 1.1 percent.
21.2 We start by writing Maclaurin series for $\cos x, \cos x=1-\frac{x^{2}}{2!}+\frac{x^{4}}{4!}-\frac{x^{6}}{6!}+\ldots$

Integrating this expression term by term yields,

$$
\int \cos x \mathrm{~d} x=\int\left(1-\frac{x^{2}}{2!}+\frac{x^{4}}{4!}+\frac{x^{6}}{6!} \ldots\right) \mathrm{d} x=x-\frac{1}{2!} \times \frac{x^{3}}{3}+\frac{1}{4!} \times \frac{x^{5}}{5}-\frac{1}{6!} \times \frac{x^{7}}{7}+\ldots+c
$$

The denominators can be tidied, by incorporating the additional factors into the factorials, $x-\frac{x^{3}}{3!}+\frac{x^{5}}{5!}-\frac{x^{7}}{7!}+\ldots+c$.
Therefore, $\int \cos x \mathrm{~d} x=x-\frac{x^{3}}{3!}+\frac{x^{5}}{5!}-\frac{x^{7}}{7!}+\ldots+c=\sin x$.
21.3 Let $\sin x=u$ and $\mathrm{e}^{-x}=\mathrm{d} v / \mathrm{d} x$. Therefore, $\mathrm{d} u / \mathrm{d} x=\cos x$ and $v=-\mathrm{e}^{-x}$ and

$$
\begin{equation*}
\int \mathrm{e}^{-x} \sin x \mathrm{~d} x=\left(-\mathrm{e}^{-x}\right) \sin x-\int\left(-\mathrm{e}^{-x}\right) \cos x \mathrm{~d} x \tag{1}
\end{equation*}
$$

The integral on the right-hand side is similar in form to the source integral. It is also a product, and can be integrated by parts, we say $\cos x=u$ and $-\mathrm{e}^{-x}=\mathrm{d} v / \mathrm{d} x$. Therefore, $\mathrm{d} u / \mathrm{d} x=$ $-\sin x$ and $v=\mathrm{e}^{-x}$. Substitution into eqn. (21.2) yields,

$$
\begin{equation*}
\int\left(-\mathrm{e}^{-x}\right) \cos x \mathrm{~d} x=\left(-\mathrm{e}^{-x}\right) \cos x-\int \mathrm{e}^{-x}(\sin x) \mathrm{d} x \tag{2}
\end{equation*}
$$

The integral on the right-hand side is the same as the original integral. Substituting for $\int\left(-\mathrm{e}^{-x}\right) \cos x \mathrm{~d} x$ from eqn. (2) into eqn. (1) yields,

$$
\int \mathrm{e}^{-x} \sin x \mathrm{~d} x=\left(-\mathrm{e}^{-x}\right) \sin x-\left(\left(-\mathrm{e}^{-x}\right) \cos x+\int \mathrm{e}^{-x} \sin x \mathrm{~d} x\right)
$$

which is readily factorized and rearranged to give,

$$
2 \int \mathrm{e}^{-x} \sin x \mathrm{~d} x=-\mathrm{e}^{-x}(\sin x+\cos x)
$$

so $\int \mathrm{e}^{-x} \sin x \mathrm{~d} x=-\frac{\mathrm{e}^{-x}}{2}(\sin x+\cos x)+c$.

Hint: It's always easier to first calculate the value of the terms inside the bracket and then multiply this answer by the factor.
21.4 Let $u=r^{2}$ and $\mathrm{d} v / \mathrm{d} r=\exp (-a r)$. Therefore, $\mathrm{d} u / \mathrm{d} r=2 r$, and $v=-\frac{1}{a} \exp (-a r)$. Inserting terms yields, $\left(r^{2} \times\left(-\frac{1}{a} \exp (-a r)\right)\right)-\left(-\frac{1}{a}\right) \int 2 r \times \exp (-a r) \mathrm{d} r$.
The integral on the right-hand side is also a product which precludes integration, so we must reduce it further. We integrate it by parts as before, saying, $2 r=u$ and $\exp (-a r)=\mathrm{d} v /$ dr . Therefore, $\mathrm{d} u / \mathrm{d} r=2$, and $v=-\frac{1}{a} \exp (-a r)=-\frac{\exp (-a r)}{a}$.
The second (intermediate) integral is,

$$
\begin{aligned}
\int 2 r \exp (-a r) \mathrm{d} r & =2 r\left(-\frac{1}{a} \exp (-a r)\right)-2\left(-\frac{1}{a}\right) \int \exp (-a r) \mathrm{d} r \\
& =2 r\left(-\frac{1}{a} \exp (-a r)\right)-2\left(\frac{1}{a^{2}} \exp (-a r)\right)
\end{aligned}
$$

The overall integral is therefore,

$$
\int r^{2} \exp (-a r) \mathrm{d} r=\left(-\frac{r^{2}}{a} \exp (-a r)\right)-\left(\frac{2 r}{a^{2}} \exp (-a r)\right)-\left(\frac{2}{a^{3}} \exp (-a r)\right)+c .
$$

We might wish to factorize for example using $a^{3}$ as a common denominator,
$-\exp (-a r)\left(\frac{a^{2} r^{2}+2 a r+2}{a^{3}}\right)+c$.

- The mathematical form $r^{2} \mathrm{e}^{-a r}$ occurs often in quantum chemistry for example when integrating volumes (see next chapter).
21.5 At first sight, we might think that we just need to substitute the limits into the expression we found for the indefinite integral in Additional Problem 21.4. This integral is, however, one of the standard integrals in the published tables, with $a=2 / a_{0}$ and $n=2$.

$$
\text { The integral that fits is, } \int_{0}^{\infty} x^{n} e^{-a x} \mathrm{~d} x=\frac{n!}{a^{(n+1)}} \text {. }
$$

$$
\text { Therefore, } \int_{0}^{\infty} r^{2} \exp \left(-\frac{2 r}{a_{0}}\right) d r=\frac{2!}{\left(2 / a_{0}\right)^{(2+1)}}=\frac{2 a_{0}^{3}}{8}=\frac{a_{0}^{3}}{4} \text {. }
$$

21.6 Let $x=u$ and $\sin 3 x=\mathrm{d} v / \mathrm{d} x$. Therefore, $\mathrm{d} u / \mathrm{d} x=1$ and $v=-1 / 3 \cos 3 x$. Inserting terms into eqn. (21.2) yields,

$$
\begin{aligned}
\int x \sin 3 x \mathrm{~d} x & =-\frac{x \cos 3 x}{3}+\int \frac{\cos 3 x}{3} \mathrm{~d} x \\
& =-\frac{x \cos 3 x}{3}+\frac{\sin 3 x}{9}+c
\end{aligned}
$$

Therefore, the solution to the overall integral is, $\frac{\sin 3 x}{9}-\frac{x \cos 3 x}{3}+c$.
21.7 Let $\ln x=u$ and let $x^{2}=\mathrm{d} v / \mathrm{d} x$. Therefore, $\mathrm{d} u / \mathrm{d} x=1 / x$ and $v=x^{3} / 3$. Inserting terms into eqn. (21.2) yields,

$$
\begin{aligned}
\int x^{2} \ln x d x & =\frac{x^{3}}{3} \ln x-\int \frac{1}{x} \times \frac{x^{3}}{3} \mathrm{~d} x \\
& =\frac{x^{3}}{3} \ln x-\int \frac{x^{3}}{3} \mathrm{~d} x \\
& =\frac{x^{3}}{3} \ln x-\frac{x^{3}}{9}+c \\
& =\frac{x^{3}}{9}(3 \ln x-1)+c
\end{aligned}
$$

21.8 This integral appears in Table 21.1 with other standard integrals.

First, we must rewrite the quotient in the form,

$$
\frac{1}{(x-a)(x-b)}=\frac{1}{a-b}\left(\frac{1}{x-a}-\frac{1}{x-b}\right) .
$$

(We can check this result by converting the terms on the right-hand side of the equation into a single fraction.)
Next, we must integrate each term,

$$
\frac{1}{a-b} \int\left(\frac{1}{x-a}-\frac{1}{x-b}\right) \mathrm{d} x
$$

Since $x>a>b$, the denominator of each term is positive and each term integrates to give a natural logarithm function,

$$
\frac{1}{a-b}(\ln (x-a)-\ln (x-b))
$$

Therefore, $\int \frac{1}{(x-a)(x-b)} \mathrm{d} x=\frac{1}{a-b} \ln \left(\frac{x-a}{x-b}\right)$
21.9 The integral that fits is, $\quad \int_{0}^{\infty} x^{n} \mathrm{e}^{-a x} \mathrm{~d} x=\frac{n!}{a^{(n+1)}}$.

We evaluate the integral, $\quad\left(\frac{4}{a_{0}^{3}}\right) \int_{0}^{\infty} r^{3} \mathrm{e}^{-2 r / a_{0}} d r=\left(\frac{4}{a_{0}^{3}}\right) \times \frac{3!}{\left(2 / a_{0}\right)^{4}}$
Thus the expectation value is, $\langle r\rangle=\left(\frac{4}{a_{0}^{3}}\right) \times \frac{6 \times a_{0}^{4}}{2^{4}}=\frac{3 a_{0}}{2}$
21.10 1. $u=\sqrt{x-4}$
2. $\mathrm{d} x / \mathrm{d} u=2 u$
so $\quad \mathrm{d} x=2 u \mathrm{~d} u$.
3. Substitute $u$ into the integral, $\int\left(\frac{u^{2}+4}{u} \times 2 u\right) \mathrm{d} u$
4. Simplifying we find,

$$
\int\left(2 u^{2}+8\right) \mathrm{d} u=\frac{2 u^{3}}{3}+8 u+c
$$

5. Converting back into a function of $x, \quad \int \frac{x}{\sqrt{x-4}} \mathrm{~d} x=\frac{2(x-4)^{\frac{3}{2}}}{3}+8(x-4)^{\frac{1}{2}}+c$
