APPENDIX D Integrals, Summations, and Calculus Results

D.1 Integrals

In this section we collect many of the nontrivial indefinite and definite integrals which may be needed for most of the derivations or exercises in the text. Some of them are evaluated using sophisticated methods (such as contour integration, discussed briefly in Section D.4), but we are only interested in using this collection as a reference. The reader is urged to consult other mathematical handbooks or especially to make use of symbolic manipulation programs such as *Mathematica*_® or *Maple*_®.

We begin by recalling that the simple rule for the differentiation of product functions

$$\frac{d}{dx}[f(x)g(x))] = \frac{df(x)}{dx}g(x) + f(x)\frac{dg(x)}{dx}$$
(D.1)

is the basis for the integration by parts (or IBP) method which we use frequently, namely

$$\int_{a}^{b} dx \, \frac{df(x)}{dx} g(x) = -\int_{a}^{b} dx f(x) \, \frac{dg(x)}{dx} + \left[f(x) \, g(x)\right]_{a}^{b} \tag{D.2}$$

Some standard indefinite integrals:

$$\int \frac{dx}{x^2 + a^2} = \frac{1}{a} \tan^{-1} \left(\frac{x}{a}\right)$$
(D.3)

$$\int \frac{dx}{a^2 - x^2} = \frac{1}{2a} \log\left(\frac{a + x}{a - x}\right) \quad (a^2 > x^2)$$
(D.4)

$$\int (\sin(ax)) (\sin(bx)) dx = \frac{\sin(a-b)x}{2(a-b)} - \frac{\sin(a+b)x}{2(a+b)} \qquad (a^2 \neq b^2)$$
(D.5)
$$\int (\cos(ax)) (\cos(bx)) dx = \frac{\sin(a-b)x}{2(a-b)} + \frac{\sin(a+b)x}{2(a+b)} \qquad (a^2 \neq b^2)$$
(D.6)

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$$\int (\sin(ax)) (\cos(bx)) \, dx = -\frac{\cos(a-b)x}{2(a-b)} - \frac{\cos(a+b)x}{2(a+b)} \qquad (a^2 \neq b^2)$$
(D.7)

$$\int dx \, x \, \sin(ax) = \frac{1}{a^2} \sin(ax) - \frac{x}{a} \cos(ax) \tag{D.8}$$

$$\int dx \, x \, \cos(ax) = \frac{1}{a^2} \cos(ax) + \frac{x}{a} \cos(ax) \tag{D.9}$$

$$\int dx \, x^2 \, \sin(ax) = \frac{2x}{a^2} \sin(ax) - \frac{(a^2 x^2 - 2)}{a^3} \cos(ax) \tag{D.10}$$

$$\int dx \, x^2 \, \cos(ax) = \frac{2x}{a^2} \cos(ax) + \frac{(a^2 x^2 - 2)}{a^3} \sin(ax) \tag{D.11}$$

$$\int dx \, x^4 \, \sin(ax) = \frac{4x(a^2x^2 - 6)}{a^4} \sin(ax) - \frac{(a^4x^4 - 12a^2x^2 + 24)}{a^5} \cos(ax)$$
(D.12)

$$\int dx \, x^4 \, \cos(ax) = \frac{4x(a^2 x^2 - 6)}{a^4} \cos(ax) + \frac{(a^4 x^4 - 12a^2 x^2 + 24)}{a^5} \sin(ax)$$
(D.13)

$$\int dx \, x \, \sin^2(ax) = \frac{x^2}{4} - \frac{x \sin(2ax)}{4a} - \frac{\cos(2ax)}{8a^2} \tag{D.14}$$

$$\int dx \, x \, \cos^2(ax) = \frac{x^2}{4} + \frac{x \sin(2ax)}{4a} + \frac{\cos(2ax)}{8a^2} \tag{D.15}$$

$$\int dx \, x^2 \, \sin^2(ax) = \frac{x^3}{6} - \left(\frac{x^2}{4a} - \frac{1}{8a^3}\right) \sin(2ax) - \frac{x \cos(2ax)}{4a^2}$$
(D.16)

$$\int dx \, x^2 \, \cos^2(ax) = \frac{x^3}{6} + \left(\frac{x^2}{4a} - \frac{1}{8a^3}\right) \sin(2ax) + \frac{x \cos(2ax)}{4a^2}$$
(D.17)

$$\int e^{ax} dx = \frac{1}{a} e^{ax} \tag{D.18}$$

$$\int x e^{ax} dx = \frac{1}{a^2} (ax - 1)e^{ax}$$
(D.19)

$$\int x^2 e^{ax} dx = \frac{1}{a^3} (a^2 x^2 - 2ax + 2)e^{ax}$$
(D.20)

Some definite integrals:

$$\int_{-\infty}^{+\infty} \frac{\sin(x)}{x} \, dx = \pi \tag{D.21}$$

$$\int_{-\infty}^{+\infty} \frac{\sin^2(x)}{x^2} \, dx = \pi \tag{D.22}$$

$$\int_{-\infty}^{+\infty} \frac{\sin^4(x)}{x^2} \, dx = \frac{\pi}{2} \tag{D.23}$$

$$\int_{-\infty}^{+\infty} \frac{(1 - \cos(x))}{x^2} \, dx = \pi \tag{D.24}$$

$$\int_{-\infty}^{+\infty} \frac{(1 - \cos(x))^2}{x^2} \, dx = \pi \tag{D.25}$$

$$\int_{-\infty}^{+\infty} \frac{\sin(x)\cos(x)}{x} dx = \frac{\pi}{2}$$
(D.26)

$$\int_{-\infty}^{+\infty} \frac{\sin(x)\cos(mx)}{x} \, dx = \begin{cases} 0 & \text{for } |m| > 1\\ \pi/2 & \text{for } |m| = 1\\ \pi & \text{for } |m| < 1 \end{cases}$$
(D.27)

$$\int_{-\infty}^{+\infty} \frac{\sin(x_1 - x)\sin(x_2 - x)}{(x - x_1)(x - x_2)} \, dx = \pi \, \frac{\sin(x_1 - x_2)}{(x_1 - x_2)} \tag{D.28}$$

$$\int_0^\infty \frac{\cos(mx)}{x^2 + a^2} \, dx = \frac{\pi}{2|a|} e^{-|ma|} \tag{D.29}$$

$$\int_0^\infty \frac{\cos(mx)\cos(nx)}{x^2 + a^2} \, dx = \frac{\pi}{a} \left(e^{-|(m-n)a|} + e^{-|(m+n)a|} \right) \tag{D.30}$$

$$\int_0^\infty \frac{\sin(mx)\sin(nx)}{x^2 + a^2} \, dx = \frac{\pi}{a} \left(e^{-|(m-n)a|} - e^{-|(m+n)a|} \right) \tag{D.31}$$

$$\int_0^\infty \cos(mx) \, e^{-ax} \, dx = \frac{a}{a^2 + m^2} \quad (a > 0) \tag{D.32}$$

$$\int_0^\infty \sin(mx) \, e^{-ax} \, dx = \frac{m}{a^2 + m^2} \quad (a > 0) \tag{D.33}$$

The following integrals make use of the Euler Gamma function ($\Gamma(z)$), the generalized factorial function, as discussed in Appendix C.9.

$$\int_{0}^{\infty} x^{n} e^{-x} dx = n! = \Gamma(n+1)$$
(D.34)

$$\int_{0}^{\infty} dx \, x^{n} \, e^{-(ax)^{m}} = \frac{1}{ma^{n+1}} \Gamma\left(\frac{n+1}{m}\right) \tag{D.35}$$

$$\int_0^1 \frac{x^m \, dx}{\sqrt{1 - x^n}} = \frac{\Gamma(1/2)\Gamma((m+1)/n)}{n\Gamma(1/2 + (m+1)/n)} \tag{D.36}$$

$$\int_{0}^{1} x^{m-1} (1-x)^{n-1} dx = \frac{\Gamma(n)\Gamma(n)}{\Gamma(m+n)}$$
(D.37)

$$\int_{0}^{\infty} \frac{x^{a} dx}{(m+x^{b})^{c}} = \frac{m^{(a+1-bc)/b}}{b} \left[\frac{\Gamma((a+1)/b)) \Gamma(c-(a+1)/b)}{\Gamma(c)} \right]$$
(D.38)

Integrals containing Gaussian terms of the form $\exp(-ax^2)$ are of special importance and we discuss their evaluation in slightly more detail. The standard trick for the evaluation of the basic integral

$$I \equiv \int_{-\infty}^{+\infty} dx \, \exp(-x^2) = \sqrt{\pi} \tag{D.39}$$

is to consider

$$I^{2} = I \cdot I = \left(\int_{-\infty}^{+\infty} dx \, \exp(-x^{2})\right) \cdot \left(\int_{-\infty}^{+\infty} dy \, \exp(-y^{2})\right)$$
$$= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx \, dy \, \exp(-x^{2} - y^{2})$$
$$= \int_{0}^{\infty} \int_{0}^{2\pi} r \, dr \, d\theta \, \exp(-r^{2})$$
$$= 2\pi \int_{0}^{\infty} dr \, r \, \exp(-r^{2})$$
$$I^{2} = \pi$$
(D.40)

so that $I = \sqrt{\pi}$. The more general basic integral is

$$I(a) = \int_{-\infty}^{+\infty} dx \, \exp(-ax^2) = \sqrt{\frac{\pi}{a}} \tag{D.41}$$

and a related one is

$$I(a, b) \equiv \int_{-\infty}^{+\infty} dx \, \exp(-ax^2 - bx)$$

= $\int_{-\infty}^{+\infty} dx \, \exp(-a(x^2 + bx/a + b^2/4a^2 - b^2/4a))$
= $\exp(b^2/4a) \int_{-\infty}^{+\infty} dx \, \exp(-a(x + b/a)^2)$

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$$I(a,b) = \exp(b^2/4a)\sqrt{\frac{\pi}{a}}$$
(D.42)

where we have used a standard method of completing the square and shifting variables. One can generalize these expressions further by "differentiating under the integral sign" to obtain

$$J(a, b; n) = \int_{-\infty}^{+\infty} dx \, x^n \exp(-ax^2 - bx)$$
$$= \left(-\frac{\partial}{\partial b}\right)^n I(a, b) = \left(-\frac{\partial}{\partial b}\right)^n \left[\exp(b^2/4a)\sqrt{\frac{\pi}{a}}\right] \qquad (D.43)$$

For example, one has

$$J(a, b; 1) \equiv \int_{-\infty}^{+\infty} x \exp(-ax^2 + bx) \, dx = \left(\frac{b}{2a}\right) \exp(b^2/4a) \sqrt{\frac{\pi}{a}} \quad (D.44)$$
$$J(a, b; 2) \equiv \int_{-\infty}^{+\infty} x^2 \exp(-ax^2 + bx) \, dx = \left(\frac{b^2 + 2a}{4a^2}\right) \exp(b^2/4a) \sqrt{\frac{\pi}{a}} \quad (D.45)$$

and so forth. For even values of n = 2k we can also evaluate J(a, b; n = 2k) by using

$$J(a,b;2k) = \int_{-\infty}^{+\infty} x^{2k} e^{-ax^2 - bx} dx = \left(-\frac{\partial}{\partial a}\right)^k I(a,b)$$
(D.46)

Integrals involving $\cos(kx)$ and $\sin(kx)$ terms and Gaussian integrands can also be done by using identities such as $\cos(kx) = [\exp(+ikx) + \exp(-ikx)]/2$ to obtain

$$\int_{-\infty}^{+\infty} e^{-ax^2 - bx} \cos(kx) \, dx = +\sqrt{\frac{\pi}{a}} \, e^{(b^2 - k^2)/4a} \, \cos(kb/2a) \tag{D.47}$$

$$\int_{-\infty}^{+\infty} e^{-ax^2 - bx} \sin(kx) \, dx = -\sqrt{\frac{\pi}{a}} \, e^{((b^2 - k^2)/4a)} \sin(kb/2a) \tag{D.48}$$

Integrals containing $ax^2 + bx + c$ arise in the study of the classical limit of the hydrogen atom and elsewhere. If we define $X = ax^2 + bx + c$ and $q = 4ac - b^2$, one has

$$\int \frac{dx}{\sqrt{X}} = -\frac{1}{\sqrt{-a}} \sin^{-1} \left(\frac{2ax+b}{\sqrt{-q}}\right) \qquad (a < 0) \tag{D.49}$$

$$\int \frac{x \, dx}{\sqrt{X}} = \frac{\sqrt{X}}{a} - \frac{b}{2a} \int \frac{dx}{\sqrt{X}}$$
(D.50)

$$\int \frac{x^2 dx}{\sqrt{X}} = \left(\frac{x}{2a} - \frac{3b}{4a^2}\right)\sqrt{X} + \frac{3b^2 - 4ac}{8a^2}\int \frac{dx}{\sqrt{X}}$$
(D.51)

$$\int \frac{x^3 dx}{\sqrt{X}} = \left(\frac{x^2}{3a} - \frac{5bx}{12a^2} + \frac{5b^2}{8a^3} - \frac{2c}{3a^2}\right)\sqrt{X} + \left(\frac{3bc}{4a^2} - \frac{5b^3}{16a^3}\right)\int \frac{dx}{\sqrt{X}}$$
(D.52)

$$\int \frac{dx}{x\sqrt{X}} = \frac{1}{\sqrt{-c}} \sin^{-1} \left(\frac{bx + 2c}{|x|\sqrt{-q}} \right) \qquad (c < 0)$$
(D.53)

D.2 Summations and Series Expansions

We collect here some useful results which evaluate the summations of certain finite and infinite series.

$$\sum_{k=1}^{k=N} x^k = \frac{1 - x^{N+1}}{1 - x} \tag{D.54}$$

$$\sum_{k=1}^{k=N} k = \frac{N(N+1)}{2}$$
(D.55)

$$\sum_{k=1}^{k=N} k^2 = \frac{N(N+1)(2N+1)}{6}$$
(D.56)

The Riemann zeta function is defined via

$$\zeta(s) = 1 + \frac{1}{2^s} + \frac{1}{3^s} + \dots = \sum_{n=1}^{\infty} \frac{1}{n^s}$$
 (D.57)

Some special cases are

$$\zeta(2) = \frac{\pi^2}{6} \qquad \zeta(4) = \frac{\pi^4}{90} \qquad \zeta(6) = \frac{\pi^6}{945} \qquad \zeta(8) = \frac{\pi^8}{9450} \qquad (D.58)$$

One can also show that

$$\zeta_{\text{odd}}(s) \equiv \frac{1}{1} + \frac{1}{3^s} + \frac{1}{5^s} + \dots = \sum_{n=1}^{\infty} \frac{1}{(2n-1)^s} = \left(1 - \frac{1}{2^s}\right) \zeta(s) \qquad (D.59)$$

so that

$$\zeta_{\text{odd}}(2) = \frac{\pi^2}{8} \quad \text{and} \quad \zeta_{\text{odd}}(4) = \frac{\pi^4}{96}$$
 (D.60)

One also has:

$$S(x) = \sum_{k=1}^{\infty} \frac{1}{((2k-1)^2 - x^2)} = \frac{\pi}{2x} \tan\left(\frac{\pi x}{2}\right)$$
(D.61)
$$T(x) = \sum_{k=1}^{\infty} \frac{1}{((2k-1)^2 - x^2)^2} = \frac{\pi}{16x^3} \left[\pi x \sec^2\left(\frac{\pi x}{2}\right) - 2\tan\left(\frac{\pi x}{2}\right)\right]$$
(D.62)

The *Taylor series expansion* of a (well-behaved) function f(x) about the point x = a is given by

$$f(x) = f(a) + f'(a)(x - a) + \frac{1}{2!}f''(a)(x - a)^2 + \cdots$$
$$= \sum_{n=0}^{\infty} \frac{f^{(n)}(a)}{n!}(x - a)^2$$
(D.63)

where

$$f^{(n)}(a) = \left. \frac{d^n f(x)}{dx^m} \right|_{x=a} \tag{D.64}$$

is the *n*th derivative of f(x) evaluated at z = a. Familiar examples include:

$$(1 \pm x)^{n} = 1 \pm nx + \frac{n(n-1)}{2!}x^{2} \pm \frac{n(n-1)(n-2)}{3!}x^{3} + \cdots$$
$$= \sum_{k=1}^{\infty} (\pm 1)^{k} \frac{n!}{(n-k)!k!}x^{k} \quad \text{for } |x| < 1$$
(D.65)

$$\sqrt{1 \pm x} = 1 \pm \frac{x}{2} - \frac{x^2}{8} \pm \frac{x^3}{16} + \dots \quad \text{for } |x| < 1$$
 (D.66)

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots = \sum_{k=0}^{\infty} \frac{x^k}{k!}$$
 for all real x (D.67)

$$\ln(1+x) = x - \frac{x}{2} + \frac{x^3}{3} + \dots = \sum_{k=1}^{\infty} (-1)^k \frac{x^k}{k} \quad \text{for } -1 < x \le +1 \quad (D.68)$$

$$\sin(x) = x - \frac{x^3}{3!} + \frac{x^5}{5!} + \dots = \sum_{k=1}^{\infty} (-1)^k \frac{x^{2k-1}}{(2k-1)!}$$
 for all real x (D.69)

$$\cos(x) = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} + \dots = \sum_{k=0}^{\infty} (-1)^k \frac{x^{2k}}{(2k)!}$$
 for all real x (D.70)

$$\tan(x) = x - \frac{x^3}{3!} + \frac{2x^5}{15} + \dots \quad \text{for } |x| < \pi/2$$
 (D.71)

A useful tool to investigate the convergence of a series expansion is the *ratio test*. If an infinite summation is defined via

$$S = \sum_{n=0}^{\infty} \rho_n \tag{D.72}$$

the limit of successive ratios is defined via

$$\rho = \lim_{n \to \infty} \frac{\rho_{n+1}}{\rho_n} \tag{D.73}$$

One then knows that

- The series *converges* (*S* is finite) if $\rho < 1$,
- The series *diverges* (*S* is infinite) if $\rho > 1$,
- The test is inconclusive (the series may either converge or diverge) if $\rho = 1$.

If the terms in the series (i) alternate in sign, (ii) decrease in magnitude (each one smaller than the one before it), and the terms approach zero, then the series is known to converge by *Liebniz's theorem*.

It is often useful to recall the definition of the (one-dimensional) integral as the "area under the curve." The trapezoidal approximation to the area under f(x) in the interval (a, b) is obtained by splitting the interval into N equal pieces of size h = (b - a)/N which gives

$$\int_{a}^{b} dx f(x) \approx F_{N}(a, b) \equiv h\left(\frac{1}{2}f(a) + \sum_{n=1}^{N-1} f(a+nh) + \frac{1}{2}f(b)\right) \quad (D.74)$$

This expression can form the basis for the simplest of numerical integration programs if necessary. The *Euler–Maclaurin formula* describes the difference between these two approximations via

$$\left[\int_{a}^{b} dx f(x)\right] - F_{N}(a,b) = -\frac{B_{2}}{2!}h^{2}f'(x)\Big|_{a}^{b} - \frac{B_{4}}{4!}h^{4}f'''(x)\Big|_{a}^{b} + \cdots \quad (D.75)$$

where the B_n are the Bernoulli numbers the first few of which are

$$B_0 = 1$$
 $B_2 = \frac{1}{6}$ $B_4 = -\frac{1}{30}$ $B_6 = \frac{1}{42}$ (D.76)

D.3 Assorted Calculus Results

The gradient-squared operator or *Laplacian operator* in rectangular (Cartesian), cylindrical (polar), or spherical coordinates is given by

$$\nabla^2 f(x, y, z) = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}$$
(D.77)

$$\nabla^2 f(r,\theta,z) = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial f}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 f}{\partial \theta^2} + \frac{\partial^2 f}{\partial z^2}$$
(D.78)

$$\nabla^{2} f(r,\theta,\phi) = \frac{1}{r^{2}} \frac{\partial}{\partial r} \left(r^{2} \frac{\partial f}{\partial r} \right) + \frac{1}{r^{2} \sin(\theta)} \frac{\partial}{\partial \theta} \left(\sin(\theta) \frac{\partial f}{\partial \theta} \right) + \frac{1}{r^{2} \sin^{2}(\theta)} \frac{\partial^{2} f}{\partial \phi^{2}}$$
(D.79)

If one changes variables in a multidimensional integral, one must also apply the appropriate transformation in the "infinitesimal measure" as well. For example, if one changes variables via

$$x, y \implies u(x, y), v(x, y)$$
 (D.80)

then one has the relation

$$du \, dv = J(w, v; x, y) \, dx \, dy = \det \left(\begin{array}{cc} \frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} \\ \frac{\partial v}{\partial x} & \frac{\partial v}{\partial y} \end{array} \right) dx \, dy \qquad (D.81)$$

with similar extensions to more dimensions; the function J(u, v; x, y) is called the *Jacobian* of the transformation. You should be able to use this approach to derive the familiar result that $dx dy dz = d\mathbf{r} = r^2 dr \sin(\theta) d\theta d\phi$.

D.4 Real Integrals by Contour Integration

Large numbers of useful real integrals, especially ones involving integration over the entire real line, can be done using simple contour integration techniques, making use of complex variables. We *very* briefly review the rudimentary complex analysis and "tricks of the trade" needed to implement many such integrals, leaving detailed discussions to undergraduate texts on mathematical methods.

The basic result from complex analysis which is required is the *residue theorem* which simplifies the evaluation of integrals of complex functions about a closed curve *C* in the complex plane, using only knowledge of the structure of the poles

(and essential singularities) that are enclosed by *C*. The appropriate connection is given by

$$\oint_C f(z) \, dz = 2\pi \, i \sum_i \, \mathcal{R}_i \tag{D.82}$$

where for a function f(z) which has a pole of order n at $z = z_0$, the residue, \mathcal{R}_i , is given by

$$\mathcal{R}_{i} = \frac{1}{(n-1)!} \left\{ \left(\frac{d}{dz} \right)^{n-1} \left[(z-z_{0})^{n} f(z) \right] \right\}_{z \to z_{0}}$$
(D.83)

The closed contour C is assumed to have a counterclockwise orientation, while if it is completed in a clockwise direction, an overall minus sign is added to the right-hand side of Eqn. (D.82). A judicious choice of an appropriate contour is often all that is needed to use the residue theorem to aid in the evaluation of integrals along the real-axis, and we present two exemplary cases.

Simple poles: Consider the real integral

$$I_1 = \int_{-\infty}^{+\infty} \frac{dx}{(1+x^2)^3}$$
(D.84)

which is clearly square-integrable and convergent. Generalize this to the complex line integral given by

$$\mathcal{I}_1 = \oint_C \frac{dz}{(1+z^2)^3}$$
(D.85)

over the contour shown in Fig. C.2(a), considering the limit that $R \to \infty$ so that the semicircle C_1 eventually extends to infinity, while the part of C along the real line reproduces I_1 . For those values on the semicircle C_1 , we can write the complex variable z in the form

$$z = Re^{i\theta}$$
 so that $dz = iRe^{i\theta} d\theta$ giving $\frac{dz}{(1+z^2)^3} \rightarrow \frac{ie^{-5i\theta}}{R^5}$ (D.86)

which becomes arbitrarily small as $R \to \infty$.

On the one hand, the complex integral over C is the sum of the desired real integral and that over the semicircular curve C_1 in the form

$$\mathcal{I}_{1} = \int_{-R}^{+R} \frac{dx}{(1+x^{2})^{3}} + \int_{C_{1}(R\to\infty)} \frac{dz}{(1+z^{2})^{2}} \longrightarrow I_{1}$$
(D.87)

in the limit that $R \to \infty$, since the contribution from C_1 vanishes. We can, however, also evaluate \mathcal{I}_1 using the residue theorem with $f(z) = 1/(1+z^2)^3$,



Figure D.1. Contours used in the evaluation of real integrals.

which has simple poles of order 3 at $z_0 = \pm i$. Using the contour *C* (semicircle C_1 plus real line) in Fig. D.1(a), which encloses the pole at $z_0 = +i$, we find

$$I_{1} = \mathcal{I}_{1} = 2\pi i \frac{1}{2!} \left\{ \left(\frac{d}{dz} \right)^{2} \left[(z - i)^{3} \frac{1}{(z - i)^{3} (z + i)^{3}} \right] \right\}_{z \to +i}$$
$$= \pi i \left(\frac{(-3)(-4)}{(2i)^{5}} \right) = \frac{3\pi}{8}$$
(D.88)

If we consider the related contour consisting of the semicircle C_2 (dashed contour) and the real line (enclosing the pole at $z_0 = -i$), we obtain the same result (recall the additional minus sign if the contour orientation is clockwise.)

Deformed contours: Consider the integral

$$I_2 = \int_{-\infty}^{+\infty} \frac{\sin(x)}{x} \, dx \tag{D.89}$$

which despite appearances is everywhere finite and convergent. The integrand is well behaved at x = 0 (since $\lim_{x\to 0} \frac{\sin(x)}{x} = 1$) and while the large |x|dependence of 1/x would yield a logarithmic divergence by itself, the alternation of signs due to the oscillatory $\frac{\sin(x)}{\sin(x)}$ gives convergence; think of the integral as an infinite sum of terms (the positive and negative areas defining the area under the integrand) with alternating signs, and of decreasing magnitude, which guarantees so-called *conditional convergence*.

In this case we choose to write I_2 in terms of the imaginary part (*Im*) of an already complex integral in the form

$$I_2 = Im\left[\int_{-\infty}^{+\infty} \frac{e^{ix}}{x} dx\right] \equiv Im[\tilde{I}]$$
(D.90)

and use contour integration over the deformed semicircle shown in Fig. C.2(b), where the region near z = 0 is treated more carefully, with a smaller semicircle of radius ϵ . The contour integral over C_1 , D_1 and the integrals over the ranges

 $(-R, -\epsilon)$ and $(+\epsilon, +R)$ constitute the desired contour *C*, but since it encloses no poles we have

$$\mathcal{I}_2 \equiv \int_C \frac{e^{iz}}{z} \, dz = 2\pi \, i \, \sum_i \mathcal{R}_i = 0 \tag{D.91}$$

via the residue theorem. The integral \mathcal{I}_2 can also be split up into the four contributions

$$\mathcal{I}_2 = \left[\int_{-R}^{-\epsilon} + \int_{+\epsilon}^{+R} \frac{e^{ix}}{x} dx\right] + \int_{C_1} \frac{e^{iz}}{z} dz + \int_{D_1} \frac{e^{iz}}{z} dz \qquad (D.92)$$

eventually taking the twin limits $\epsilon \to 0$ and $R \to \infty$. The first two terms give \tilde{I} in this limit, while for C_1 we use the same parameterization as in Eqn. (D.86) and it is easy to show that the contribution is exponentially suppressed as $\exp(-R\sin(\theta))$ as $R \to \infty$. Finally, for the contribution around D_1 , we use $z = \epsilon \exp(i\theta)$ which gives

$$\int_{D_1} \frac{e^{iz}}{z} dz = \int_{\pi}^0 \frac{e^{i\epsilon e^{i\theta}}}{\epsilon e^{i\theta}} \left(i\epsilon e^{i\theta} d\theta \right) \longrightarrow i \int_{\pi}^0 d\theta = -i\pi$$
(D.93)

as $\epsilon \to 0$. From Eqns (D.91) and (D.92) we then find that $0 = I_2 = \tilde{I} + 0 - i\pi$ so that

$$\int_{-\infty}^{+\infty} \frac{e^{ix}}{x} dx = \tilde{I} = i\pi \quad \text{and} \quad I_2 = Im[\tilde{I}] = Im[i\pi] = \pi \tag{D.94}$$

A large number of other similar integrals can be done using the deformed contour shown in Fig. C.2(b). For example, you should be able to show that

$$\int_{-\infty}^{+\infty} \frac{[1 - \cos(y)]}{y^2} \, dy = \pi \tag{D.95}$$

by taking the real part of a related integral, and extending it to the contour used above.

D.5 Plotting

The functional relationship between two variables is often best exemplified or analyzed (or even discovered in the first place) by plotting the "data" in an appropriate manner. In this section, we briefly recall some of the basics of plotting techniques; because linear relations are easiest to visualize, many standard tricks rely on graphing data in such a way as to yield a straight line. For variables which are connected by an exponential relation one has

exponential:
$$y = ae^{bx} \implies \ln(y) = \ln(a) + bx$$
 (D.96)

which suggests that one plot ln(y) versus *x*; this gives a so-called *semilog plot*. A straight-line fit on such a plot implies an exponential relation, and the "generalized slope" is given by

$$b = \frac{(\ln(y_2) - \ln(y_1))}{(x_2 - x_1)} = \frac{\ln(y_2/y_1)}{(x_2 - x_1)}$$
(D.97)

The value of *a* (or $\ln(a)$) plays the role of an "intercept" and can be extracted from any point on the line once *b* is known; if the point with x = 0 is included, then y(0) = a is the most obvious choice.

For power-law relations of the form

power-law:
$$y = cx^d \implies \ln(y) = \ln(c) + d\ln(x)$$
 (D.98)

it is best to graph ln(y) versus ln(x) giving a *log–log plot* where the "generalized slope" is now

$$d = \frac{(\ln(y_2) - \ln(y_1))}{(\ln(x_2) - \ln(x_1))} = \frac{\ln(y_2/y_1)}{\ln(x_2/x_1)}$$
(D.99)

D.6 Problems

- PD.1. Derive any of the integrals in Eqns (D.5)–(D.7) by using complex exponentials.
- PD.2. Derive any of the integrals in Eqns (D.8)–(D.11) using IBP techniques.
- PD.3. Derive the integral in Eqn. (D.8) by differentiating both sides of the relation

$$\int \cos(ax) \, dx = \frac{1}{a} \sin(ax) \tag{D.100}$$

with respect to *a*.

- **PD.4.** Evaluate J(a, b; n) in Eqn. (D.43) for n = 2, 4 by differentiating with respect to *b*. Then evaluate those two cases using Eqn. (D.46) by differentiating with respect to *a* and confirm you get the same answers.
- **PD.5.** Derive Eqn. (D.59).
- PD.6. Evaluate the integral in Eqn. (D.24) using contour integration.
- **PD.7.** At very low temperatures, the heat capacity (at constant volume) of metals is expected to given by an expression of the form

$$C_V = \gamma T + AT^3 \tag{D.101}$$

Given experimental values for *T* and $C_V(T)$, what would be the best way to plot the data to confirm such a relation and to most easily extract γ and *A*?