

# Exercises of *The Mathematica GuideBook for Symbolics*

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## CHAPTER 1

### Exercises

#### 1.<sup>L2</sup> The 2 in the Factorization of $x^i - 1$ , Heron's Formula, Volume of Tetrahedron, Circles of Apollonius, Circle ODE, Modular Transformations, Two-Point Taylor Expansion, Quotiential Derivatives

a) Program a function which finds all  $i$  for which numbers other than 0 or  $\pm 1$  appear as coefficients of  $x^j$  ( $0 \leq j \leq i$ ) in the factorized decomposition of  $x^i - 1$  ( $1 \leq i \leq 500$ ) [591★]. Do not use temporary variables (no Block or Module constructions).

b) Let  $P_1, P_2$ , and  $P_3$  be three points in the plane. Starting from the formula  $A = |(P_2 - P_1) \times (P_3 - P_1)|/2$  for the area  $A$  of the triangle formed by  $P_1, P_2$ , and  $P_3$ , derive a formula for the area which only contains the lengths of the three sides of the triangle (Heron's area formula).

c) Let  $P_1, P_2, P_3$ , and  $P_4$  be four points in  $\mathbb{R}^3$ . Starting from the formula  $V = (\text{areaOfOneFace height} / 3)$  for the volume  $V$  of the tetrahedron formed by  $P_1, P_2, P_3$ , and  $P_4$ , derive a formula for the volume which only contains the lengths of the six edges of the tetrahedron [849★].

d) Given are three circles in the plane that touch each other pairwise. In the "middle" between these three circles now put a fourth circle that touches each of the three others. Calculate the radius of this circle as an explicit function of the radius of the three other circles (see [1642★], [420★], [157★], [1695★], [847★], and [700★]).

e) Calculate the differential equation that governs all circles in the  $x,y$ -plane (from I.I.5.6 of [904★]).

f) Show that the three equations

$$\begin{aligned}u^4 - v(u)^4 - 2 u v(u) (1 - u^2 v(u)^2) &= 0 \\u^6 - v(u)^6 + 5 v(u)^2 u^2 (u^2 - v(u)^2) - 4 u v(u) (1 - u^4 v(u)^4) &= 0 \\(1 - u^8)(1 - v(u)^8) - (1 - u v(u))^8 &= 0\end{aligned}$$

are solutions of the (so-called modular) differential equation [1449★]

$$\left( \left( \frac{1+k^2}{k-k^3} \right)^2 - \left( \frac{1+l}{l-l^3} \right)^2 l'(k)^2 \right) l'(k)^2 + 3 l''(k)^2 - 2 l'(k) l'''(k) = 0.$$

The change of variables between  $\{k, l\}$  and  $\{u, v\}$  is given by  $k^{\frac{1}{4}} = u$  and  $l^{\frac{1}{4}} = v$ .

g) The function

$$w(x) = c_1 e^{-\int \frac{f(x)}{1-h(x)} dx} \left( c_2 + \int \frac{e^{\int g(x) dx + \int \frac{f(x)}{1-h(x)} dx}}{1-h(x)} dx \right)$$

fulfills a linear second-order differential equation [705★]. Derive this differential equation.

h) Prove the following two identities (from [1854★] and [905★]):

$$\begin{aligned} \tan\left(\frac{1}{4} \tan^{-1}(4)\right) &= 2 \left( \cos\left(\frac{6\pi}{17}\right) + \cos\left(\frac{10\pi}{17}\right) \right) \\ \cos\left(\frac{\pi}{7}\right) &= \frac{1}{6} + \frac{\sqrt{7}}{6} \left( \cos\left(\frac{1}{3} \cos^{-1}\left(\frac{1}{2\sqrt{7}}\right)\right) + \sqrt{3} \sin\left(\frac{1}{3} \cos^{-1}\left(\frac{1}{2\sqrt{7}}\right)\right) \right) \end{aligned}$$

i) Given a rectangular box of size  $w_1 \times h_1 \times d_1$ . Is it possible to put a second box of size  $w_2 \times h_2 \times d_2$  in the first one such that  $1/w_2 + 1/h_2 + 1/d_2$  is equal to, less than, or greater than  $w_1 + h_1 + d_1$ ?

j) What geometric object is described by the following three inequalities?

$$|\phi x| + |y| < 1 \wedge |\phi y| + |z| < 1 \wedge |x| + |\phi z| < 1$$

( $\phi$  is the Golden ratio.)

k) Check the following integral identity [1073★]:

$$\int_0^\xi \left( \int_x^\infty \frac{f(t)}{t} dt \right)^2 dx = \int_0^\xi \left( \frac{1}{x} \int_0^x f(t) dt \right)^2 dx + \left( \sqrt{\xi} \int_\xi^\infty \frac{f(t)}{t} dt + \frac{1}{\sqrt{\xi}} \int_0^\xi f(t) dt \right)^2.$$

l) Check the following identity [1916★] for small integer  $n$  and  $r$ :

$$\begin{aligned} \sum_{k=1}^n \frac{p(a_k)}{(x-a_k)^{r+1} \prod_{l \neq k}^n (a_k - a_l)} = \\ \frac{(-1)^r}{r! \prod_{k=1}^n (x-a_k)} \left( p^{(r)}(x) + \sum_{j=1}^r (-1)^j \binom{r}{j} p^{(r-j)}(x) A \left( \sum_{i=1}^n (x-a_i)^{-1}, \sum_{i=1}^n (x-a_i)^{-2}, \dots, \sum_{i=1}^n (x-a_i)^{-j} \right) \right) \end{aligned}$$

Here  $p(z)$  is a polynomial of degree equal to or less than  $n$ ; the  $a_k$  are arbitrary complex numbers and the multivariate polynomials  $A(\tau_1, \dots, \tau_j)$  are defined through

$$A(\tau_1, \tau_2, \dots, \tau_j) = \sum_{\substack{k_1, k_2, \dots, k_j \\ k_1 + 2k_2 + \dots + jk_j = j}} \frac{j!}{k_1! k_2! \dots k_j!} \left( \frac{\tau_1}{1} \right)^{k_1} \left( \frac{\tau_2}{2} \right)^{k_2} \dots \left( \frac{\tau_j}{j} \right)^{k_j}.$$

m) Given five points in  $\mathbb{R}^2$ , find all relations between the oriented areas (calculated, say, with the determinantal formula from Subsection 1.9.2) of the nine triangles that one can form using the points.

n) Is it possible to position six points  $P_1, \dots, P_6$  in the plane in such a way that they have the following integer distances between them [820★]?

	$P_1$	$P_2$	$P_3$	$P_4$	$P_5$	$P_6$
$P_1$	0	87	158	170	127	68
$P_2$	87	0	85	127	136	131
$P_3$	158	85	0	68	131	174
$P_4$	170	127	68	0	87	158
$P_5$	127	136	131	87	0	85
$P_6$	68	131	174	158	85	0

o) Show that there are no  $3 \times 3$  Hadamard matrices [79★], [1882★], [686★]. (An  $n \times n$  Hadamard matrix  $\mathbf{H}_n$  is a matrix with elements  $\pm 1$  that fulfills  $\mathbf{H}_n \cdot \mathbf{H}_n^T = n \mathbf{1}_n$ .)

p) The two-point Taylor series of order for a function  $f(z)$  analytic in  $z_1, z_2$  is defined through [1169★]

$$f(z) = \sum_{n=0}^o (c_n(z_1, z_2)(z - z_1) + c_n(z_2, z_1)(z - z_2))(z - z_1)^n (z - z_2)^n + R_{o+1}(z, z_1, z_2).$$

Here  $R_{o+1}(z, z_1, z_2)$  is the remainder term and the coefficients  $c_n(z_1, z_2)$  are given as

$$c_0(z_1, z_2) = \frac{f(z_2)}{z_2 - z_1}$$

$$c_n(z_1, z_2) = \sum_{k=0}^n \frac{(k + n - 1)!}{k! n! (n - k)!} \frac{(-1)^k k f^{(n-k)}(z_1) + (-1)^{n+1} n f^{(n-k)}(z_2)}{(z_1 - z_2)^{k+n+1}}.$$

Calculate the two-point Taylor series  $\mathcal{T}_{0,2\pi}^{(20)}[\sin](z)$  of order 20 for  $f(z) = \sin(z)$ ,  $z_1 = 0$ , and  $z_2 = 2\pi$ . Find  $\max_{z_1 \leq z \leq z_2} |f(z) - \mathcal{T}_{20}(z)|$ .

q) While for a smooth function  $y(x)$ , the relation  $dy(x)/dx = 1/(dx(y)/dy)$  holds; the generalization  $d^n y(x)/dx^n = 1/(d^n x(y)/dy^n)$  for  $n \geq 2$  in general does not hold. Find functions  $y(x)$  such that the generalization holds for  $n = 2$  [247★]. Can you find one for  $n = 3$ ?

r) Define a function (similar to the built-in function D) that implements the quotential derivatives  $q^n./qx^n$  of a function  $f(x)$  defined recursively by [1308★]

$$\frac{q^n f(x)}{dx^n} = \frac{q}{qx} \left( \frac{q^{n-1} f(x)}{dx^{n-1}} \right)$$

with the first quotential derivatives  $q./qx$  defined as

$$\frac{q^1 f(x)}{qx^1} = \frac{qf(x)}{qx} = \lim_{q \rightarrow 1} \ln \left( \frac{f(qx)}{f(x)} \right).$$

Show that  $qf(y(x))/qx = qf(y(x))/qy \cdot qy(x)/qx$ .

Define the multivariate quotential derivative recursively starting with the rightmost ones, meaning

$$\frac{q^2 f(x, y)}{qx qy} = \frac{q}{qx} \left( \frac{qf(x, y)}{qy} \right).$$

Show by explicit calculation that

$$\frac{qf(x, y)}{qy} \frac{q^2 f(x, y)}{qx qy} = \frac{qf(x, y)}{qx} \frac{q^2 f(x, y)}{qy qx}.$$

s) Conjecture the value of the following sum:  $\sum_{k=1}^{\infty} (\prod_{j=1}^k a_{j-1} / (x + a_j))$ . Here  $a_0 = 1$ ,  $a_k \in \mathbb{C}$ ,  $a_k \neq 0$ ,  $x \neq 0$  [1660★].

t) Show that the solutions  $x(X, Y, Z)$ ,  $y(X, Y, Z)$ , and  $z(X, Y, Z)$  of Bateman's homework problem [132★]

$$\left( \begin{array}{ccc} \frac{\partial x(X, Y, Z)}{\partial X} & \frac{\partial y(X, Y, Z)}{\partial X} & \frac{\partial z(X, Y, Z)}{\partial X} \\ \frac{\partial x(X, Y, Z)}{\partial Y} & \frac{\partial y(X, Y, Z)}{\partial Y} & \frac{\partial z(X, Y, Z)}{\partial Y} \\ \frac{\partial x(X, Y, Z)}{\partial Z} & \frac{\partial y(X, Y, Z)}{\partial Z} & \frac{\partial z(X, Y, Z)}{\partial Z} \end{array} \right) = k(X, Y, Z)$$

are given (implicitly) by [314★], [1047★]

$$x = \frac{\partial \Phi(X, y, z)}{\partial y}$$

$$\frac{\partial \Phi(X, y, z)}{\partial X} = \frac{\partial \Psi(X, Y, z)}{\partial z}$$

$$\frac{\partial \Psi(X, Y, z)}{\partial Y} = \int k(X, Y, Z) dZ.$$

The two functions  $\Phi(X, y, z)$  and  $\Psi(X, Y, z)$  are arbitrary and fulfill  $\partial^2 \Phi(X, y, z) / (\partial X \partial y) \neq 0$  and  $\partial^2 \Psi(X, Y, z) / (\partial Y \partial z) \neq 0$ .

## 2.<sup>L1</sup> Horner's Form, Bernoulli Polynomials, Squared Zeros, Polynomialized Radicals, Zeros of Icosahedral Equation, Iterated Exponentials, Matrix Sign Function, Appell–Nielsen Polynomials

a) Given a polynomial  $p(x)$ , rewrite it in Horner's form.

b) Bernoulli polynomials  $B_n(x)$  are uniquely characterized by the property  $\int_x^{x+1} B_n(t) dt = x^n$ . Use this method to implement the calculation of Bernoulli polynomials  $B_n(x)$ . Try to use only built-in variables (with the exception of  $x$  and  $n$ , of course).

c) Given the polynomial  $x^4 + a_3 x^3 + a_2 x^2 + a_1 x + a_0$  with zeros  $x_1, x_2, x_3$ , and  $x_4$ , calculate the coefficients (as functions of  $a_0, a_1, a_2$ , and  $a_3$ ) of a polynomial that has the zeros  $x_1^2, x_2^2, x_3^2$ , and  $x_4^2$ .

d) Express the real zeros of

$$-1 + x + 2\sqrt{1+x^2} - 3\sqrt[3]{1+x^3} + 5\sqrt[5]{1+x^5} - 4 = 0$$

as the zeros of a polynomial.

e) Show that all nontrivial solutions of  $x^{10} + 11x^5 - 1 = 0$  stay invariant under the following 60 substitutions:

$$x \rightarrow \epsilon^i x$$

$$x \rightarrow -\frac{\epsilon^i}{x}$$

$$x \rightarrow \frac{\epsilon^j (\epsilon^i + x (\epsilon^4 + \epsilon))}{x - \epsilon^i (\epsilon^4 + \epsilon)}$$

$$x \rightarrow -\frac{\epsilon^j (x - \epsilon^i (\epsilon^4 + \epsilon))}{\epsilon^i + x (\epsilon^4 + \epsilon)}$$

**f)** Iterated exponentials  $\exp(c_1 z \exp(c_2 z \exp(c_3 z \cdots)))$  can be used to approximate functions [975★], [1897★], [1898★], [47★]. Find values for  $c_1, c_2, \dots, c_{10}$  such that  $\exp(c_1 z \exp(c_2 z \exp(c_3 z \cdots)))$  approximates the function  $1 + \ln(1 + z)$  around  $z = 0$  as best as possible.

**g)** Motivate symbolically the result of the following input.

```
m = Table[1/(i + j + 1), {i, 5}, {j, 5}];
```

```
FixedPoint[ (# + Inverse[#])/2&, N[m], 100]
```

**h)** Efficiently calculate the list of coefficients of the polynomial

$$(x^4 + x^3 + x^2 + x + 1)^{500} (x^2 + x + 1)^{1000} (x + 1)^{2000}$$

without making use of any polynomial function like `Expand`, `Coefficient`, `CoefficientList`, ...

**i)** What is the minimal distance between the roots of  $z^3 + c^2 z + 1 = 0$  for real  $c$ ?

**j)** Let  $f^{(k)}(z) = f(f^{(k-1)}(z))$ ,  $f^{(1)}(z) = f(z) = z^2 - c$ . Then the following remarkable identity holds [1146★], [120★]:

$$\exp\left(-\sum_{k=1}^{\infty} c_k \frac{z^k}{k}\right) = 1 + \sum_{k=1}^{\infty} \frac{\left(\frac{z}{2}\right)^k}{\prod_{j=1}^k f^{(j)}(0)}$$

where

$$c_k = \sum_{j=1}^{2^k} \frac{1}{f^{(k)'}(z_j) (f^{(k)'}(z_j) - 1)}.$$

The sum appearing in the definition of the  $c_k$  extends over all  $2^k$  roots of  $f^{(k)}(z) = z$ . Expand both sides of the identity in a series around  $z = 0$  and check the equality of the terms up to order  $z^4$  explicitly.

**k)** Write a one-liner that, for a given integer  $m$ , quickly calculates the matrix of values

$$c_{e,d} = \lim_{x \rightarrow 0} \frac{\partial^d \left( \frac{x}{\sin(x)} \right)^e}{\partial x^d}$$

for  $1 \leq e \leq m$ ,  $0 \leq d \leq m$ .

**l)** The Appell–Nielsen polynomials  $p_n(z)$  are defined through the recursion  $p_n'(z) = p_{n-1}(z)$ , the symmetry constraint  $p_n(z) = (-1)^n p_n(-z - 1)$ , and the initial condition  $p_0(z) = 1$  [327★], [1352★]. Write a one-liner that calculates the first  $n$  Appell–Nielsen polynomials. Visualize the polynomials.

**m)** Write a one-liner that uses `Integrate` (instead of the typically used `D`) to derive the first  $n$  terms of the Taylor expansion of a function  $f$  around  $x$  that is based on the following identity [734★], [554★]

$$f(x+h) = \sum_{k=0}^{n-1} \frac{h^k}{k!} f^{(k)}(x) + \int_0^h \int_0^{h_1} \cdots \int_0^{h_{n-1}} f^{(n)}(x+h_n) dh_n \dots dh_2 dh_1.$$

**n)** A generalization of the classical Taylor expansion of a function  $f(x)$  around a point  $x_0$  into functions  $\varphi_k(x)$ ,  $k = 0, 1, \dots, n$  (where the  $\varphi_k(x)$  might be other functions that the monomials  $x^k$ ) can be written as [1855★]

$$f(x) \approx -\frac{1}{W(\varphi_0(x_0), \dots, \varphi_n(x_0))} \begin{pmatrix} 0 & \varphi_0(x) & \varphi_1(x) & \cdots & \varphi_n(x) \\ f(x_0) & \varphi_0(x_0) & \varphi_1(x_0) & \cdots & \varphi_n(x_0) \\ f'(x_0) & \varphi_0'(x_0) & \varphi_1'(x_0) & \cdots & \varphi_n'(x_0) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ f^{(n)}(x_0) & \varphi_0^{(n)}(x_0) & \varphi_1^{(n)}(x_0) & \cdots & \varphi_n^{(n)}(x_0) \end{pmatrix}.$$

Here the  $W(\varphi_0(\xi), \dots, \varphi_n(\xi))$  is the Wronskian of the  $\varphi_0(\xi), \dots, \varphi_n(\xi)$  and it is assumed not to vanish at  $x_0$ . Implement this approximation and approximate  $f(x) = \cos(x)$  around  $x_0 = 0$  through  $\exp(x), \exp(x/2), \dots, \exp(x/m)$ . Can this formula be used for  $m = 25$ ?

o) Show that the function [1233★]

$$w(z) = \frac{((u(z) + 2z u'(z))^2 - 4z u'(z)^2)^2}{8(u(z) u'(z) (u(z) + 2(z-1) u'(z)) (u(z) + 2z u'(z)))}$$

where  $u(z) = c_1 f_1(z) + c_2 f_2(z)$  and  $f_{1,2}(z)$  are solutions of  $(1-z)z f''(z) + (1-2z) f'(z) - f(z)/4 = 0$  fulfills the following special case of the Painlevé VI equation:

$$w''(z) = \frac{1}{2} \left( \frac{1}{w(z)} + \frac{1}{w(z)-1} + \frac{1}{w(z)-z} \right) w'(z)^2 - \left( \frac{1}{z} + \frac{1}{z-1} + \frac{1}{w(z)-z} \right) w'(z) + \frac{w(z)(w(z)-1)(w(z)-z)}{2(z-1)^2 z^2} \left( \frac{z(z-1)}{(w(z)-z)^2} + 4 \right).$$

### 3.<sup>L1</sup> Nested Integration, Derivative [-n], PowerFactor, Rational Painlevé II Solutions

a) Given that the following definition is plugged into *Mathematica*, what will be the result of `f[2][x]`?

```
f[n_][x_] := Integrate[f[n - 1][x - z], {z, 0, x}]
```

```
f[0][x_] = Exp[-x];
```

Consider the evaluation process. How would one change the first two inputs to get the “correct” result as if from

```
Nest[Integrate[# /. {x -> x - z}, {z, 0, x}] &, Exp[-x], 2]
```

b) Find two (univariate) functions  $f$  and  $g$ , such that `Integrate[f, x] + Integrate[g, x]` gives a different result than does `Integrate[f + g, x]`. Find a (univariate) functions  $f$  and integration limits  $x_l, x_m$ , and  $x_u$ , such that `Integrate[f, {x, x_l, x_u}]` gives a different result than does `Integrate[f, {x, x_l, x_m}] + Integrate[f, {x, x_m, x_u}]`.

c) What does the following code do?

```
Derivative[i_Integer?Negative][f_] :=
With[{pI = Integrate[f[C], C]},
  derivative[i + 1][Function[pI] /. C -> #] /;
  FreeQ[pI, Integrate, {0, Infinity}]]
```

Predict the results of `Derivative[+4][Exp[1 #] &]` and `Derivative[-4][Exp[1 #] &]`.

d) Is it possible to find a function  $f(x, y)$  such that `D[Integrate[f(x, y), x], y]` is different from `Integrate[D[f(x, y), y], x]`?

e) Write a function `PowerFactor` that does the “reverse” of the function `PowerExpand`. It should convert products of radicals into one radical with the base having integer powers. It should also convert sums of logarithms into one logarithm and  $s \log(a)$  into  $\log(a^s)$ .

f) The rational solutions of  $w''(z) = 2w(z)^3 - 4zw(z) + 4k$ ,  $k \in \mathbb{N}^+$  (a special Painlevé II equation) can be expressed in the following way [976★], [919★], [1226★], [961★]:

Let the polynomials  $q_k(z)$  be defined by the generating function  $\sum_{k=0}^{\infty} q_k(z) \xi^k = \exp(z\xi + \xi^3/3)$  (for  $k < 0$ , let  $q_k(z) = 0$ ).

Let the determinants  $\sigma_k(z)$  be defined by matrices  $(a_{ij})_{0 \leq i, j \leq k-1}$  with  $a_{ij} = q_{k+i-2j}(z)$  (for  $k = 0$ , let  $\sigma_0(z) = 1$ ). Then,  $w_k(z)$  is given as  $w_n(z) = \partial \log(\sigma_{k+1}(z)/\sigma_k(z))/\partial z$ . Calculate the first few  $w_k(z)$  explicitly.

#### 4.<sup>L1</sup> Differential Equations for the Product, Quotient of Solutions of Linear Second-Order Differential Equations

Let  $y_1(z)$  and  $y_2(z)$  be two linear independent solutions of

$$y''(z) + f(z)y'(z) + g(z)y(z) = 0$$

The product  $u(z) = y_1(z)y_2(z)$  obeys a linear third-order differential equation

$$u'''(z) + a_p[f(z), g(z)]u''(z) + b_p[f(z), g(z)]u'(z) + c_p[f(z), g(z)]u(z) = 0$$

The quotient  $w(z) = y_1(z)/y_2(z)$  obeys (Schwarz's differential operator; see, for instance, [855★] and [1922★])

$$w'''(z)w'(z) + a_q[f(z), g(z)]w''(z)^2 + b_q[f(z), g(z)]w'(z)^2 = 0$$

Calculate  $a_p, b_p, c_p$  and  $a_q, b_q$ . (For analogous equations for the solutions of higher-order differential equations, see [1034★].)

#### 5.<sup>L1</sup> Singular Points of ODEs, Integral Equation

a) First-order ordinary differential equations of the form  $y'(x) = P(x, y)/Q(x, y)$  possess singular points  $\{x_i^*, y_i^*\}$  [217★], [1414★], [1761★], [1116★], [472★], [958★]. These are defined by  $P(x_i^*, y_i^*) = Q(x_i^*, y_i^*) = 0$ . It is possible to trace the typical form of the solution curves in the neighborhood of a singular point by solving  $y'(x) = (ax + by)/(cx + dy)$ . Some typical forms include the following examples:

$$\text{a knot point } y'(x) = \frac{2y(x)}{x}, \quad y'(x) = \frac{y(x)+x}{x}, \quad y'(x) = \frac{y(x)}{x}$$

$$\text{a vortex point } y'(x) = -\frac{y(x)}{x}$$

$$\text{an eddy point } y'(x) = \frac{y(x)-x}{y(x)+x}$$

Investigate which of the given differential equations can be solved analytically by *Mathematica*, and plot the behavior of the solution curves in a neighborhood of the singular point  $\{0, 0\}$ .

b) Consider the general case (meaning  $\lambda$  is a regular value) of the Fredholm integral equation of the second kind

$$y(x) - \lambda \int_a^b \mathcal{K}(x, \xi) y(\xi) d\xi = f(x)$$

with a separable kernel (meaning  $\mathcal{K}(x, \xi)$  can be written in the form  $\mathcal{K}(x, \xi) = \sum_{j=1}^n g_j(x) h_j(\xi)$ ). Implement a function that solves such Fredholm integral equations in the classical manner, by forming and solving a linear system in the  $r_j = \int_a^b h_j(\xi) y(\xi) d\xi = \int_a^b h_j(x) y(x) dx$ .

The solution  $y(x)$  can be written in the form  $y(x) = f(x) + \lambda \int_a^b \Gamma(x, \xi) f(\xi) d\xi$  with the resolvent kernel  $\Gamma(x, \xi)$ .

Implement a function that calculates the truncated form of the Fredholm resolvent [1640★], [1438★], [1466★], [1900★], [1113★], [628★]

$$\Gamma^F(x, \xi) = \frac{D(x, \xi; \lambda)}{D(\lambda)}$$

$$D(x, \xi; \lambda) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \lambda^k d_k(x, \xi), \quad D(\lambda) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \lambda^k c_k.$$

where the  $c_k$  and  $d_k(x, \xi)$  are recursively defined through

$$c_0 = 1, \quad c_k = \int_a^b d_{k-1}(\xi, \xi) d\xi$$

$$d_0(\xi, \xi) = \mathcal{K}(\xi, \xi), \quad d_k(x, \xi) = c_k \mathcal{K}(x, \xi) - k \int_a^b \mathcal{K}(x, \rho) d_{k-1}(\rho, \xi) d\rho.$$

Finally, implement a function that calculates a truncated form of the Neumann form of the resolvent (valid for a limited set of  $\lambda$ ) that utilizes iterated kernels.

$$\Gamma^N(x, \xi) = \sum_{k=1}^{\infty} \lambda^k \mathcal{K}_k(x, \xi)$$

$$\mathcal{K}_1(x, \xi) = \mathcal{K}(x, \xi), \quad \mathcal{K}_n(x, \xi) = \int_a^b \mathcal{K}(x, \rho) \mathcal{K}_{n-1}(\rho, \xi) d\rho.$$

Use the implemented functions to solve the equation  $y(x) - \lambda \int_0^1 \sin(x + \xi) y(\xi) d\xi = \cos(x)$  exactly and up to  $O(\lambda^5)$ .

## 6.<sup>L1</sup> Inverse Sturm–Liouville Problems, Graeffe Method

a) In recent years, so-called “inverse problems” have assumed an increasingly important role (see, e.g., [326★], [782★], [723★], [1902★], [1534★], [93★], and [163★]). Very roughly speaking, they are as follows: For a given result, find the associated problem that led to the result. For Sturm–Liouville eigenvalue problems

$$-y''(x) + v(x)y(x) = \lambda y(x)$$

with given eigenvalues  $\lambda_i$ , the solutions are completely known. We consider the following special case: Given eigenvalues  $\lambda_1, \dots, \lambda_n$  of the problem

$$-y_i''(x) + v(x)y_i(x) = \lambda_i y_i(x), \quad y_i(0) = 0, \quad 0 \leq x \leq \infty$$

find one (eigenvalue-independent) potential that leads to these eigenvalues (given only finitely many eigenvalues, of course, infinitely many solutions exist). The following method solves this problem constructively:



$$\begin{aligned}\varphi_0(x, \lambda) &= \frac{\sin(\lambda x)}{\lambda} \\ u(x)_{ij} &= \delta_{ij} + \int_0^x \varphi_0(s, \sqrt{\lambda_j}) \varphi_0(s, \sqrt{\lambda_i}) ds \quad i, j = 1, 2, \dots, n \\ v(x) &= -2 \frac{d^2 \ln(\det U(x))}{dx^2}.\end{aligned}$$

Here,  $U(x)$  is a matrix with matrix elements  $u_{ij}(x)$ . Then, the corresponding (normalizable) eigenfunctions  $\psi_i(x)$  are given by

$$\psi_i(x) = \sum_{j=1}^n u_{ij}^{-1}(x) \varphi_0(x, \sqrt{\lambda_j})$$

Implement these formulas, and for  $n = 1$ , verify that the resulting  $v(x)$  and  $\psi_1(x)$  satisfy the equation

$$-\psi_1''(x) + v(x) \psi_1(x) = \lambda_1 \psi_1(x)$$

Plot the result for  $n = 2$ . For details see [1674★], [1261★], [1901★], [325★], [1769★], [860★], [553★], [881★], [33★], [1591★], [1562★], [1386★], [1810★], [409★], [324★], and [1457★]. For the vector-valued version, see [345★].

a) Implement the Graeffe method [837★], [886★], [1197★], [1198★], [1667★] to calculate the roots of the polynomial  $p = z^5 + 5z^4 - 10z^3 - 10z^2 + 5z + 2 = 0$  to 100 digits. The Graeffe method calculates the polynomials

$$\begin{aligned}p_{n+1}(z^2) &= p_n(z) p_n(-z) \\ p_0(z) &= p.\end{aligned}$$

The distinct real roots  $z_k$  of the polynomial  $p$  of degree  $d$  are then given by

$$|z_k| = \lim_{n \rightarrow \infty} \left| \frac{a_{n,k-1}}{a_{n,k}} \right|^{2^{-n}}$$

where  $p_{n+1}(z) = \sum_{k=0}^d a_{n,k} z^k$ .

### 7.<sup>L3</sup> Finite Element Method: Lagrange and Hermite Interpolation

This problem is meant for readers who are familiar with the finite element method (FEM). This is not the right place to give a detailed account of the method itself. Interested readers should consult any typical FEM book, such as [1114★], [377★], [278★], [1599★], [83★], [84★], [85★], [551★], [136★], [805★], [1780★], [31★], and [142★] for some computer algebra applications. For applications in physics, see, for example, [789★], [1325★], [1066★], [1478★], [241★], [845★], [14★], [1048★], [1139★], [1601★], [13★], and [729★], and the references therein.

a) Suppose we are given an elliptic partial differential equation of second order in two space dimensions

$$\frac{\partial^2 u(x, y)}{\partial x^2} + \frac{\partial^2 u(x, y)}{\partial y^2} + \lambda u(x, y) = f(x, y)$$

For most finite-element calculations, it is common to use Lagrange basis functions of the first or second order on triangles. Higher-order elements may be needed in some applications to get higher accuracy (say up to eighth order in some applications [804★]). To carry out the calculation, we need to compute the corresponding stiffness matrices, element vectors, and, for eigenvalue problems, the corresponding mass matrices. These should be computed for the case of linear isoparametric maps of the unit triangle onto arbitrary triangles. (If this mapping is nonlinear, this will not be possible, in general, without using numerical integration.) To accomplish this, solve the following subproblems:

- Compute and plot the position of the data points for Lagrange interpolation [474★], [1160★]. Usually, the data points are numbered as follows: The three outer vertices are given the numbers 1, 2, and 3. Now starting with vertex 1, continue in a spiral winding in the same sense as 1, 2, 3 to the center.
- Compute the Lagrange shape functions of  $n$ th-order for the unit triangle.
- Program a corresponding integration routine to efficiently compute integrals of the form

$$\int_0^1 \int_0^{1-\xi} \xi^p \eta^q d\eta d\xi = \frac{p! q!}{(p+q+2)}$$

- Compute the element vectors, the mass matrices, and the stiffness matrices for various orders.
- b) Now, consider the 1D case. The Hermite element functions  $\chi_{k,l}^{(p,d)}(\xi)$  are defined through their smooth interpolation property

$$\left. \frac{\partial^n \chi_{k,l}^{(p,d)}(\xi)}{\partial \xi^n} \right|_{\xi=\xi_m} = \delta_{k,m} \delta_{l,n}.$$

Here  $p+1$  indicates the number of nodes in one cell and the index  $d$  indicates the order of smoothness. The two integer labels  $k$  and  $l$  range over  $0 \leq k \leq p$  and  $0 \leq l \leq d$ , and  $\xi$  runs from 0 to 1. (In most cases, one uses equidistantly spaced  $\xi_m$ , meaning  $\xi_m = m/p$ .)

Consider the eigenvalue problem for a harmonic oscillator [1696★], [566★], [1467★], [1468★], [1770★]

$$\begin{aligned} -\psi_j''(x) + x^2 \psi_j(x) &= \varepsilon_j \psi_j(x) \\ \psi(-\infty) &= \psi(\infty) = 0 \end{aligned}$$

with the exact eigenvalues  $\varepsilon_j = 2j+1$ ,  $j \in \mathbb{N}$ . Discretize the problem in the interval  $[-L, L]$  into  $e$  elements and use the ansatz

$$\psi_j(x) = \sum_{j=0}^{e-1} \sum_{k=0}^p \sum_{l=0}^d c_{k,l}^{(j,p,d)} \chi_{k,l}^{(p,d)}(\xi(x)) \theta(x-x_j) \theta(x_{j+1}-x).$$

Here  $\xi(x) = (x-x_j)/\delta$ ,  $x_j = -L + j/e\delta$ ,  $\delta = 2L/e$  and the Dirichlet boundary conditions enforce  $c_{0,0}^{(0,p,d)} = c_{0,0}^{(e-1,p,d)} = 0$ . Continuity and smoothness at the leftmost and rightmost nodes enforces  $c_{p,l}^{(j,p,d)} = c_{0,l}^{(j+1,p,d)}$  for  $1 \leq j \leq j-2$ .

Construct the algebraic eigenvalue problem corresponding to the minimization problem

$$\int_{-L}^L \left( \left( \frac{\partial \psi_j(x)}{\partial x} \right)^2 + (x^2 - \varepsilon_j) \psi_j(x) \right) dx$$

and calculate the lowest eigenvalues.

Is it possible to get the lowest eigenvalue correct to 20 digits with resulting matrices of dimension  $64 \times 64$  or less?

### 8.<sup>L2</sup> Helium Atom, Improved Variational Method

a) In 1933, Hylleraas and Undheim ([895★], see also [169★], [1293★], [652★], [1383★], and [862★]) published the results of a variational calculation [1843★] of the ground-state ( ${}_2S$  state) energy  $\lambda_0(k_{\min}, c_{\min})$  of an (ortho) Helium atom [1001★]. Without going into the physical background (see [1260★], or for more depth, see [170★], [1072★], [1460★], [1035★], [1409★], [1570★], [896★], [827★], [78★], [1063★], [1060★], [1728★], [1297★], [742★], [1346★], [1384★], [1920★], [1538★], and [1717★], and the references therein), we present the underlying mathematical problem.

Find the smallest zero  $\lambda_0(k, c)$  of the determinant of the  $6 \times 6$  matrix  $D$  with elements  $D_{ij}$  defined below. (The minimum is around  $k_{\min} \approx 0.5, c_{\min} \approx 0.5$ .) The experimental value of the ground-state energy is  $-1.08762$ . How well does the calculation perform?

$$\begin{aligned}
 D_{ij} &= \lambda N_{ij}(c) + k(L_{ij}(c) + L'_{ij}(c)) - k^2 M_{ij}(c) \\
 N_{ij}(c) &= \int_0^\infty ds \int_0^s du \int_0^u dt \frac{u(s^2 - t^2)}{8} \varphi_i \varphi_j \\
 L_{ij}(c) &= \int_0^\infty ds \int_0^s du \int_0^u dt 2 s u \varphi_i \varphi_j \\
 L'_{ij}(c) &= \int_0^\infty ds \int_0^s du \int_0^u dt \frac{(s^2 - t^2)}{4} \varphi_i \varphi_j \\
 M_{ij}(c) &= \int_0^\infty ds \int_0^s du \int_0^u dt (u(s^2 - t^2) (\varphi_{i,s} \varphi_{j,s} + \varphi_{i,t} \varphi_{j,t} + \varphi_{i,u} \varphi_{j,u}) + \\
 &\quad s(u^2 - t^2) (\varphi_{i,s} \varphi_{j,u} + \varphi_{i,u} \varphi_{j,s}) + t(s^2 - u^2) (\varphi_{i,t} \varphi_{j,u} + \varphi_{i,u} \varphi_{j,t})).
 \end{aligned}$$

Here are the  $\varphi_i(u, s, t)$ :

$$\begin{aligned}
 \varphi_1(u, s, t) &= e^{-s/2} \sinh(ct/2) \\
 \varphi_2(u, s, t) &= s \varphi_1(u, s, t) \\
 \varphi_3(u, s, t) &= t e^{-s/2} \cosh(ct/2) \\
 \varphi_4(u, s, t) &= u \varphi_1(u, s, t) \\
 \varphi_5(u, s, t) &= u \varphi_2(u, s, t) \\
 \varphi_6(u, s, t) &= u \varphi_3(u, s, t).
 \end{aligned}$$

$\varphi_{i,s}$  is the partial derivative  $\partial \varphi_i(u, s, t) / \partial s$ , and the analogous formula holds for  $\varphi_{i,t}$  and  $\varphi_{i,u}$ .

b) A possible scheme for improving variational calculations with one variational parameter is the following (see [1689★] and [1921★]): Given a (real) trial function  $\psi_0(\beta; x)$  in which  $\beta$  is the variational parameter, one constructs additional functions (which we take here orthonormalized)  $\psi_1(\beta; x), \psi_2(\beta; x)$ , and so on (all depending on the same parameter  $\beta$ ) via

$$\begin{aligned}
 \psi_i(\beta; x) &= \frac{\partial \psi_{i-1}(\beta; x)}{\partial \beta} \\
 \int_L \psi_i^2(\beta; x) dx &= 1.
 \end{aligned}$$

(Here, the integration extends over the range where the  $\psi_0(\beta; x)$  are defined.) As the trial function, it uses

$$\Psi(\beta; x) = \sum_{i=0}^n c_i(\beta) \psi_i(\beta; x).$$

For the eigenvalue problem for a hermitian operator  $H$ ,  $H(x)\psi(x) = \varepsilon\psi_i(x)$ , the condition for  $\varepsilon(\beta)$  to be the best approximation to the lowest eigenvalue becomes

$$\det |H_{ij}(\beta) - \varepsilon(\beta) M_{ij}(\beta)| = 0$$

Here,  $H_{ij}(\beta)$  and  $M_{ij}(\beta)$  (which reflects the nonorthogonality of the  $\psi_i(\beta; x)$ ) are defined as

$$H_{ij}(\beta) = \int_L \psi_i(\beta; x) H(x) \psi_j(\beta; x) dx$$

$$M_{ij}(\beta) = \int_L \psi_i(\beta; x) \psi_j(\beta; x) dx.$$

Carry out the above calculations for the following particular realizations of the described scheme [1921★] in  $L = (-\infty, \infty)$ :

$$H = -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} x^2 + x^4$$

$$\psi_0(\beta; x) = \sqrt{\frac{\beta}{\sqrt{\pi}}} e^{-\beta^2 \frac{x^2}{2}}.$$

Use different techniques to calculate explicit numerical values for the lowest eigenvalue for  $n \leq 6$ . The so-defined  $\varepsilon(\beta)$  has to be minimized with respect to  $\beta$ .

## 9.<sup>L2</sup> Hyperspherical Coordinates, Constant Negative Curvature Surface

a) The standard  $n$ -dimensional spherical coordinates are defined by the following relations [1757★], [189★] (for nonstandard  $n$ -dimensional spherical coordinates, see [1350★]):

$$\begin{aligned} x_1 &= r \cos \vartheta_1 \\ x_2 &= r \sin \vartheta_1 \cos \vartheta_2 \\ x_3 &= r \sin \vartheta_1 \sin \vartheta_2 \cos \vartheta_3 \\ &\vdots \\ x_{n-1} &= r \sin \vartheta_1 \sin \vartheta_2 \cdots \sin \vartheta_{n-2} \cos \vartheta_{n-1} \\ x_n &= r \sin \vartheta_1 \sin \vartheta_2 \cdots \sin \vartheta_{n-2} \sin \vartheta_{n-1}. \end{aligned}$$

Here, the  $x_i$  are Cartesian coordinates. Compute and simplify the Jacobian of this coordinate transformation for the first  $n$ . Compare the times needed by `Simplify` with the times needed by manual simplification.

b) The following gives a parametric description of a family of constant negative curvature [1763★] surfaces [1241★] ( $0 < c < 1$  is the family parameter) [1513★], [1583★], [1584★], [1514★], [1585★].

$$\mathbf{r}(u, v) = \{0, 0, x\} + \frac{2d \cosh(cx) \sin(dy)}{c \mathcal{D}} \{\sin(y), -\cos(y), 0\} +$$

$$\frac{2d^2 \cosh(cx) (\cosh^2(cx) - \sin^2(dy))}{c \mathcal{D} \tilde{\mathcal{D}}} \{\cos(y) \cos(dy), \sin(y) \cos(dy), -\sinh(cx)\}$$

$$\mathcal{D} = d^2 \cosh^2(cx) + c^2 \sin^2(dy)$$

$$\tilde{\mathcal{D}} = \cos^2(dy) \cosh^2(cx) + \sin^2(dy) \sinh^2(cx)$$

$$c = \sqrt{1 - d^2}$$

$$x = u + v, y = u - v$$

Show that  $\mathbf{r}(u, v)$  has a constant curvature  $\mathcal{K}$ . The curvature  $\mathcal{K}$  can be calculated through the following formulas.

$$\mathcal{K} = \frac{1}{|\mathbf{n}|^2} \frac{eg - f^2}{\mathcal{E}\mathcal{G} - \mathcal{F}^2}$$

$$\mathcal{E} = \frac{\partial \mathbf{r}(u, v)}{\partial u} \cdot \frac{\partial \mathbf{r}(u, v)}{\partial u}, \quad \mathcal{G} = \frac{\partial \mathbf{r}(u, v)}{\partial v} \cdot \frac{\partial \mathbf{r}(u, v)}{\partial v}, \quad \mathcal{F} = \frac{\partial \mathbf{r}(u, v)}{\partial u} \cdot \frac{\partial \mathbf{r}(u, v)}{\partial v}$$

$$e = \frac{\partial^2 \mathbf{r}(u, v)}{\partial u^2} \cdot \mathbf{n}, \quad f = \frac{\partial^2 \mathbf{r}(u, v)}{\partial u \partial v} \cdot \mathbf{n}, \quad g = \frac{\partial^2 \mathbf{r}(u, v)}{\partial v^2} \cdot \mathbf{n}$$

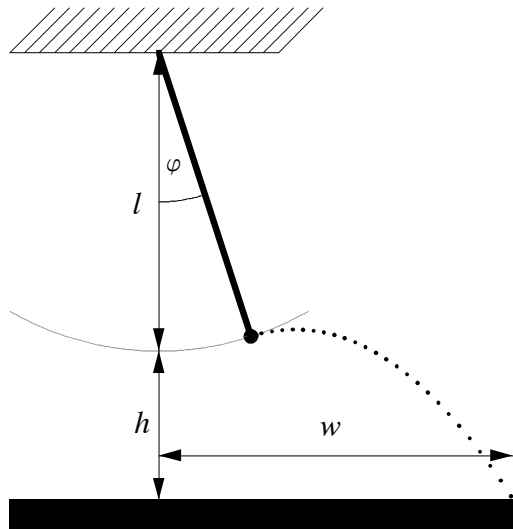
$$\mathbf{n} = \frac{\partial \mathbf{r}(u, v)}{\partial u} \times \frac{\partial \mathbf{r}(u, v)}{\partial v}$$

Visualize some of the surfaces of the family.

### 10.<sup>L2</sup> Throw from a Finite Height, Pendulum Throw, Spring System

a) Determine the optimal throw angle (optimal with respect of achieving the furthest possible throw distance) for a throw starting from a finite height  $h$ . Visualize the optimality of this angle. Calculate the envelope of all throw curves for a variable throw angle [510★], [667★], [109★], [77★], [511★], [636★].

b) Consider a mathematical pendulum with mass  $m$ , length  $l$ , and minimum height  $h$  above the ground. Suppose during the movement of the pendulum that the string is suddenly cut. The subsequent trajectory of the mass is a parabola. Determine the angle of release  $\varphi$  for which the point of contact  $x_s = w$  of the pendulum with the horizontal floor is farthest. Try to find an analytic solution. The horizontal distance is measured from the abscissa of the point from which the pendulum is hung, and the angle  $\varphi$  is measured from the vertical. The maximum angle should be less than  $\pi/2$ . Plot the solution.



c) Take a Platonic solid and replace all edges by springs of identical stiffness and the vertices with point masses. For small elongations, analyze the “breathing mode” (meaning all vertices move radial and in phase) of the resulting structure. How many normal modes contribute to the “breathing mode” and how does its frequency compare with other eigenmodes.

### 11.<sup>L1</sup> Sturm–Liouville Problems in Normal Form

The general eigenvalue problem for a linear differential equation of second order takes the form

$$f_2(x) y''(x) + f_1(x) y'(x) + (f_0(x) + \lambda g(x)) y(x) = 0.$$

Often, it is useful to rewrite this eigenvalue problem in the Liouville normal form

$$\eta''(\xi) + (\lambda + \nu(\xi))\eta(\xi) = 0.$$

In this form, we can better determine the  $\nu(\xi)$  for which there is an analytical solution of the problem (see [113★], [1533★], [1302★], [27★], [653★], [1276★], [128★], [1333★], [1180★], [138★], and [1859★]; for multidimensional analytic solutions, see [1797★]). This transformation is given by (we assume sufficient smoothness for the corresponding functions)

$$\begin{aligned}\eta(\xi) &= \Phi(x)y(x) \\ \xi &= \xi(x) = \int^x \sqrt{\frac{g(x)}{f_2(x)}} dx \\ \Phi(x) &= \sqrt[4]{\frac{g(x)}{f_2(x)}} \exp\left(\frac{1}{2} \int^x \frac{f_1(x)}{f_2(x)} dx\right).\end{aligned}$$

Determine the resulting  $\nu(\eta)$ , and implement this transformation. Try to generate error messages when the function is called with inappropriate arguments.

## 12.<sup>L1</sup> Noncentral Collision, Bernstein Polynomials, Bernstein Operator

a) A sphere of mass  $M$  is at rest at the point  $\{0, 0\}$ . Suppose a second sphere (of the same diameter) with velocity  $\{v_x, v_y\}$  collides with the first one in an elastic noncentral collision. Suppose the coordinates of the center of the second sphere at the time of collision are  $\{x, y\}$ . Compute the velocity of both spheres after of the collision, and plot their motion. Suppose the momentum, energy, and angular momentum conservation laws hold (the angular momentum law implies that no tangential forces are present).

b) Calculate a closed form of the envelope of the scaled maxima  $n^{1/2} x_m$  of the Bernstein polynomials  $b_{n,k}(x) = \sum_{k=0}^n \binom{n}{k} x^k (1-x)^{n-k}$ ,  $0 \leq k \leq n$  as  $n \rightarrow \infty$  [1183★].

c) The eigenvectors of the Bernstein operator  $\hat{B}_n$

$$\hat{B}_n(f(x)) = \sum_{k=0}^n \binom{n}{k} x^k (1-x)^{n-k} f\left(\frac{k}{n}\right)$$

are polynomials of degree less than or equal to  $n$ . Find the eigenvectors for  $n = 36$  and visualize them in the interval  $0 \leq x \leq 1$ .

## 13.<sup>L2</sup> A Sensitive Linear System of Equations, Bisector Surface, Surface Connecting Three Cylinders, Double Torus Surface

a) Suppose we are given the following linear inhomogeneous system of equations [1541★]:

$$\begin{aligned}- 367296 t - 43199 u + 519436 v - 954302 w &= 1 \\ 259718 t - 477151 u - 367295 v - 1043199 w &= 1 \\ 886731 t + 88897 u - 1254026 v - 1132096 w &= 1 \\ 627013 t + 566048 u - 886732 v + 911103 w &= 0.\end{aligned}$$

How many digits are needed to be sure that the solution is correct to 10 digits? How sensitive to a small change of the coefficients is the solution of this system? (See also [747★] and [1491★].)

b) The bisector surface of two geometrical objects (points, lines, surfaces) is the set of points that have the same distance to each of the two geometrical objects [616★], [572★], [571★], [615★], [1032★], [164★], [573★], [1417★], [825★]. Calculate the

implicit form of the bisector surface of a torus and a point in generic position. Visualize the bisector surface for the point at the center of the torus.

c) Construct a polynomial surface  $p(x, y, z) = 0$  that in a smooth way connects the three half-infinite cylinders [117★], [1874★], [634★], [631★], [1827★], [339★], [1825★] given by their parametric representations

$$\begin{aligned} \{x, \cos(\varphi), \sin(\varphi)\} & \quad 0 \leq \varphi \leq 2\pi, 3 \leq x < \infty \\ \{\cos(\varphi), y, \sin(\varphi)\} & \quad 0 \leq \varphi \leq 2\pi, 3 \leq y < \infty \\ \{\cos(\varphi), \sin(\varphi), z\} & \quad 0 \leq \varphi \leq 2\pi, 3 \leq z < \infty. \end{aligned}$$

Make a picture of that part of the polynomial  $p(x, y, z) = 0$  that connects the three cylinders and the three cylinders themselves.

d) Calculate the implicit form of a polynomial surface of a double torus, such that the two holes of the double torus tightly enclose the hole of the given torus with radii  $r = 1$  and  $R = 3$ , and the given torus tightly encloses the “middle bridge” of the double torus.

#### 14.<sup>L2</sup> Transformation of Variables in a PDE, $\det(e^{\mathbf{A}}) = e^{\text{Tr}\mathbf{A}}$ , Matrix Derivative, Lewis–Carroll Identities

a) Program a function `DerivativeVariableTransformation` that carries out transformations of variables in expressions that contain partial derivatives. Starting with Cartesian coordinates, use it to transform  $\Delta f(x, y, z)$  into spherical coordinates.

b) Given the result of evaluating the following determinant.

`A = Array[a, {3, 3}]; Det[MatrixExp[A]]`

By virtue of  $\det(e^{\mathbf{A}}) = e^{\text{Tr}\mathbf{A}}$  this simplifies to `Exp[a[1, 1] + a[2, 2] + a[3, 3]]`. Use *Mathematica* to carry out this simplification.

c) Construct a one-liner that proves the matrix identity

$$\frac{\mathbf{1}}{\mathbf{1} - \lambda \mathbf{A}} = \sum_{k=0}^{\infty} \lambda^k \mathbf{A}^k$$

for a generic symbolic  $3 \times 3$  matrix  $\mathbf{A}$ .

d) The differential quotient  $d_{\mathbf{H}}(t, \mathbf{A})$  of the matrix exponential  $\exp(t\mathbf{A})$  in (matrix) direction  $\mathbf{H}$  is defined as [1324★], [1499★], [1753★], [1705★]

$$d_{\mathbf{H}}(t, \mathbf{A}) = \lim_{\varepsilon \rightarrow 0} \frac{e^{t(\mathbf{A} + \varepsilon \mathbf{H})} - e^{t\mathbf{A}}}{\varepsilon}.$$

$d_{\mathbf{H}}(t, \mathbf{A})$  can be expressed in the following way:

$$d_{\mathbf{H}}(t, \mathbf{A}) = \int_0^t e^{(t-\tau)\mathbf{A}} \mathbf{H} e^{\tau\mathbf{A}} d\tau.$$

For  $n = 2$ , show the equivalence of the two expressions for  $d_{\mathbf{H}}(t, \mathbf{A})$  by explicit calculation.

f) Take a generic  $3 \times 3$  matrix  $\mathcal{A}$  and the resulting 81 matrices of size  $2 \times 2$  that arise from extracting two columns and two rows from  $\mathcal{A}$  and the 9 matrices of size  $1 \times 1$  that arise from using one columns and one row from  $\mathcal{A}$ . Find algebraic relations that are obeyed by the determinants of these 91 matrices.

### 15.<sup>L2</sup> $1 + 2 + 3 + \dots = -1/12$ , Casimir Effect

- a) Often, in physics books and journals, one sees the following sum:  $1 + 2 + 3 + \dots = -1/12$  [1141★], [577★], [186★], [1211★]. Motivate this finite result for this divergent sum.
- b) Calculate the following expression (the order of the limits matter):

$$\lim_{\lambda \rightarrow 0} \lim_{m \rightarrow \infty} \left( \sum_{n=0}^m n^3 e^{-\lambda n} - \int_0^m x^3 e^{-\lambda x} dx \right)$$

- c) Consider the following formally divergent expression [1578★], [1919★], [230★] (arising from the classical limit of the Casimir effect)

$$\mathcal{A}(l, L) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \left( \ln \left( \frac{\sqrt{\frac{\pi^2 n^2}{l^2} + k_x^2 + k_y^2}}{\sqrt{\frac{\pi^2 n^2}{(L/2)^2} + k_x^2 + k_y^2}} \right) + \ln \left( \frac{\sqrt{\frac{\pi^2 n^2}{(L-l)^2} + k_x^2 + k_y^2}}{\sqrt{\frac{\pi^2 n^2}{(L/2)^2} + k_x^2 + k_y^2}} \right) \right) dk_x dk_y.$$

Find a finite result for  $\mathcal{A}(l, L)$ .

### 16.<sup>L2</sup> Random Functions, Use of Numerical Techniques

- a) Implement a function (of one variable) `RandomFunction` that produces a random function (of a given depths  $n$ ) sometimes involving trigonometric functions, sometimes power functions, sometimes trigonometric functions of power functions, .... Use such a random function to find an integral that could be done, but *Mathematica* is not able to do it.
- b) Find at least ten functions discussed in this chapter that, when called with purely symbolic input (this means input with infinite precision), potentially make internal use of numerical techniques. Show convincingly that these functions really use approximative numbers internally.
- c) Find all built-in functions for which `Derivative[2][function]` evaluates to a nontrivial result.

### 17.<sup>L3</sup> Thomas–Fermi Equation, Yoccoz Function, $y(x) = x/\ln(x)$ Inversion, Lagrange–Bürmann Theorem, Divisor Sums, Multiple Differentiation

- a) Iteratively compute the first few terms of a series expansion of a solution  $f(x)$  of the differential equation

$$f''(x) = \frac{\sqrt{f(x)^3}}{\sqrt{x}}$$

satisfying the initial conditions

$$f(0) = f_0, f'(0) = f_{s0}$$

(This is the differential equation for the radial electron density distribution of atoms in the Thomas–Fermi approximation. For details on the Thomas–Fermi approximation, see [748★], [118★], [1657★], [673★], [1391★], [524★], [494★], [1729★], [1730★], [587★], [1214★], [1213★], [1037★], [1131★], [146★], [319★], [963★], [1303★], [589★], [627★], and [869★].)

- b) Carrying out the Majorana substitution  $\{x, \varphi(x)\} \rightarrow \{t, u(t)\}$  defined through [593★], [594★], [595★]



$$t = \frac{1}{\sqrt[6]{144}} \sqrt{x} \sqrt[6]{\varphi(x)}$$

$$u(t) = -\sqrt[3]{\frac{16}{3}} \frac{\varphi'(x)}{\sqrt[3]{\varphi(x)^4}}$$

in the Thomas–Fermi equation  $\varphi''(x) = x^{-1/2} \varphi(x)^{3/2}$  yields a first-order differential equation for  $u(t)$ . Derive this differential equation for  $u(t)$ .

c) The Yoccoz function [1218★], [1893★]  $u(z)$  is the limit  $u(z) = \lim_{n \rightarrow \infty} u_n(z)$  of the polynomials

$$u_0(z) = 1$$

$$u_n(z) = u_{n-1}(z) - \frac{z^{n-1}}{2} u_{n-1}^2(z).$$

Calculate the first 100 terms of the expansion of  $u(z)$  around  $z = 0$ :

$$u(z) = \sum_{k=0}^{\infty} c_k z^k.$$

Is the calculation of the first 1000 terms feasible? Make a graphic of  $\arg(u(0.999 e^{i\varphi}))$  and conjecture some properties of  $\arg(u(r e^{i\varphi}))$  as  $r \rightarrow 1^-$ .

d) The inverse function  $x(y)$  to  $y(x) = x/\ln(x)$  can be asymptotically for  $x \rightarrow \infty$ , expressed in the form (see [193★], [397★], [649★], [859★], [933★], and [125★])

$$x(y) = y \ln(y) + y \ln(\ln(y)) + y \sum_{i=1}^{\infty} \sum_{j=1}^i a_{ij} \frac{(\ln(\ln(y)))^j}{\ln^i(y)}.$$

Determine the coefficients  $a_{ij}$  for  $i, j < 5$ .

e) Calculate the series expansion up to order three of  $g(z) = \tan(z)$  if  $z = z(w)$  is defined as the inverse function of  $\exp(z) + \ln(z+1)$  around  $z_0 = 1$ . Calculate the result one time directly and one time using the Lagrange–Bürmann theorem [1853★], [1500★], [335★], [894★], [305★], [1628★], [1659★], [1694★]. It states that if  $w = f(z)$ ,  $w_0 = w(z_0)$ ,  $w'(z_0) \neq 0$ , the series expansion of  $g(f^{-1}(w))$  around  $w_0$  is given by

$$g(f^{-1}(w)) = g(z_0) + \sum_{i=1}^{\infty} \frac{1}{i!} \left[ \frac{d^{i-1}}{d\xi^{i-1}} \left( g'(\xi) \left( \frac{\xi - z_0}{f(\xi) - w_0} \right)^i \right) \right]_{\xi=z_0} (w - w_0)^i$$

Determine the coefficients  $a_{ij}$  for  $i, j < 5$ .

f) Using the three functions

$$P(q) = 1 - 24 \sum_{k=1}^{\infty} \frac{k q^k}{1 - q^k}$$

$$Q(q) = 1 + 240 \sum_{k=1}^{\infty} \frac{k^3 q^k}{1 - q^k}$$

$$Q(q) = 1 - 504 \sum_{k=1}^{\infty} \frac{k^5 q^k}{1 - q^k},$$

it is possible to express many sums of the form [1469★], [1795★]

$$S_{\alpha,o}(q) = \sum_{k=1}^{\infty} k^{\alpha} \sigma_o(k) q^k$$

( $\sigma_o(k)$  being the divisor sum function) as polynomials in  $P(q)$ ,  $Q(q)$ , and  $R(q)$ . Find at least ten such polynomials.

**g)** The Eisenstein series  $\mathcal{E}_n(q)$ , defined by

$$\mathcal{E}_n(q) = 1 - \frac{2n}{B_n} \sum_{k=1}^{\infty} \sigma_{n-1}(k) q^k$$

(where  $B_n$  are the Bernoulli numbers and  $\sigma_n(k)$  are the divisor sums) fulfill identities of the form [726★], [710★]

$$\sum_{m=1}^o \prod_{k=1}^{l^{(m)}} c_{m,k} \mathcal{E}_{n_k^{(m)}}(q)^{e_k^{(m)}} = 0$$

with integer  $c_m, k$ . In the last identity, the indices  $n_k^{(m)}$  and the exponents  $e_k^{(m)}$  fulfill the constraint

$$\sum_{k=1}^{l^{(m)}} n_k^{(m) e_k^{(m)}} = d, \quad m = 1, \dots, o$$

where  $d$  is a given positive even integer. Examples of such relations are  $\mathcal{E}_4(q)^2 - \mathcal{E}_8(q) = 0$  and  $250 \mathcal{E}_6(q)^2 + 441 \mathcal{E}_4(q) \mathcal{E}_8(q) - 691 \mathcal{E}_{12}(q) = 0$ . Based on comparing coefficients of powers of  $q$ , implement a search for such identities and find at least ten.

**h)** The polynomials  $S_k(x)$  defined by

$$S_k(x) = \frac{1}{k+1} \sum_{j=0}^k (-1)^j \binom{k+1}{j} B_j x^{k+1-j}$$

(here  $B_j$  are the Bernoulli numbers) have the property  $S_k(n) = \sum_{j=1}^n j^k$ . In addition, they fulfill identities of the form [1490★]

$$S_k(x)^2 = \sum_{j=0}^{2o+1} c_j S_j(x).$$

Implement a one-liner that calculates this identity for a given  $k$ .

**i)** Consider the following infinite product representation of the function  $\exp$  [1756★]:

$$e^z = \prod_{k=1}^{\infty} \frac{1 - a_k z^k}{1 + a_k z^k}.$$

Calculate the first 100 of the  $a_k$ . How good an approximation of  $e$  (meaning  $z = 1$ ) results from this? What is the radius of convergence of this infinite product?

j) Given a vector-valued differential equation  $x'_i(s) = f_i(x_1(s), \dots, x_n(s))$ , the higher derivatives  $\frac{\partial^2 x_i(s)}{\partial s^2}$ ,  $\frac{\partial^3 x_i(s)}{\partial s^3}$ , ... can be expressed as functions of partial derivatives of the  $f_i$  with respect to the  $x_j$ s. Using the convention that a sum is understood over all doubly occurring subscripts and that  $f_{i;j,k,\dots}$  stands as a shortcut for  $\frac{\partial^n f_i(s)}{\partial x_j \partial x_k \dots}$ , the derivatives can be concisely written as  $\frac{\partial x_i(s)}{\partial s} = f_i$ ,  $\frac{\partial^2 x_i(s)}{\partial s^2} = f_{i;j} f_j$ ,  $\frac{\partial^3 x_i(s)}{\partial s^3} = f_{i;j,k} f_j f_k + f_{i;j} f_{j;k} f_k$ , ... [663★]. Calculate explicit expressions for the first six  $\frac{\partial^n x_i(s)}{\partial s^n}$ . Write the result in the most concise form by renaming dummy summation indices.

### 18.L3 Trig Values in Radicals, Ramanujan Identities, Modular Transformation

a) If possible, compute exact values (containing only square and cube roots and no exponentials and logarithms) for  $\cos(j\pi/n)$  and  $\sin(j\pi/n)$  (let  $2 < n < 10$  and  $j < n/2$ ).

b) Write a program that expresses every trigonometric function with argument  $p/q\pi$  ( $p, q$  integer) that can be expressed as a function containing only addition, subtraction, multiplication, division, and square rooting. (Do not use the function `FunctionExpand`.)

c) Prove the following three identities that are from Ramanujan [160★]:

$$\frac{\sin(2\pi/7)}{\sin^2(3\pi/7)} - \frac{\sin(\pi/7)}{\sin^2(2\pi/7)} + \frac{\sin(3\pi/7)}{\sin^2(\pi/7)} = 2\sqrt{7}$$

$$\frac{\sin^2(2\pi/7)}{\sin^4(3\pi/7)} + \frac{\sin^2(\pi/7)}{\sin^4(2\pi/7)} + \frac{\sin^2(3\pi/7)}{\sin^4(\pi/7)} = 28$$

$$\begin{aligned} & \frac{\sin^2(3\pi/7)}{\sin^4(\pi/7)} \left( 2 \frac{\sin(2\pi/7)}{\sin(3\pi/7)} + 4 \frac{\sin(3\pi/7)}{\sin(\pi/7)} \right) + \\ & \frac{\sin^2(\pi/7)}{\sin^4(2\pi/7)} \left( -2 \frac{\sin(3\pi/7)}{\sin(\pi/7)} + 4 \frac{\sin(\pi/7)}{\sin(2\pi/7)} \right) - \\ & \frac{\sin^2(2\pi/7)}{\sin^4(3\pi/7)} \left( 2 \frac{\sin(\pi/7)}{\sin(2\pi/7)} + 4 \frac{\sin(2\pi/7)}{\sin(3\pi/7)} \right) = 280. \end{aligned}$$

After making the following substitutions, for which  $n$  do these identities remain true?

$$\begin{aligned} \sin(\pi/7) & \rightarrow \sin(n\pi/7) \\ \sin(2\pi/7) & \rightarrow \sin(2n\pi/7) \\ \sin(3\pi/7) & \rightarrow \sin(3n\pi/7). \end{aligned}$$

d) Determine all transformations of the form (modular transformations [1807★], [1838★])

$$y(x, k) = \frac{\alpha(k) + \beta(k)x}{\alpha'(k) + \beta'(k)x}$$

such that the following equation holds:

$$\left(\frac{\partial y(x, k)}{\partial x}\right)^2 = \frac{1}{M(k)} \frac{(1 - y(x, k)^2)(1 - l(k)^4 y(x, k)^2)}{(1 - x^2)(1 - k^4 x^2)}$$

Calculate all corresponding  $l(k)^4$  and  $M(k)$ . Represent the results in a “nice” form.

### 19.L2 Forced Damped Oscillation, $(1 + z/n)^n$ -Series, e-Series, q-Logarithm

a) Suppose we are given the differential equation of a 1D oscillation subject to a harmonic force [64★]

$$m x''(t) + \gamma x'(t) + k x(t) = F_0 \cos(\omega t)$$

Compute the series expansion (in  $\gamma$ ) of the maximum of the  $n$ th derivative (with respect to  $\omega$ ) of the amplitude of the resulting oscillation in the forced state.

If in addition to the external force  $F_0 \cos(\omega t)$ , a stochastic force  $\mathcal{F}(t)$  with the properties  $\langle \mathcal{F}(t) \rangle = 0$  and  $\langle \mathcal{F}(t) \mathcal{F}(t') \rangle = 2 \gamma k_B T \delta(t - t')$  ( $\langle \cdot \rangle$  indicates time averaging) acts on the oscillator, the motion of the oscillator becomes different for each realization of the force  $\mathcal{F}(t)$ . Averaging over all realizations yields the probability distribution [332★], [1300★], [130★]

$$W(x, t; x_0, v_0) = \frac{1}{\sqrt{4 \pi q I_{\psi\psi}(t)}} \exp\left(-\frac{(x - x_c(t; x_0, v_0))^2}{4 \pi q I_{\psi\psi}(t)}\right)$$

for the probability to find the oscillator as position  $x$  at time  $t$  if the oscillator started at time 0 at position  $x_0$  with velocity  $v_0$ .

Here  $q = \gamma k_B T / m$ ,  $I_{\psi\psi}(t) = \int_0^t \psi(\tau)^2 d\tau$ ,  $\psi(\tau) = (e^{\mu_1(t-\tau)} - e^{\mu_2(t-\tau)}) / (\mu_1 - \mu_2)$ ,  $\mu_{1/2} = -\gamma/2 \pm (\gamma^2/4 - \omega_0^2)^{1/2}$ ,  $\omega_0 = (k/m)^{1/2}$ , and  $x_c(x, t; x_0, v_0)$  is the solution of the oscillator ODE with initial conditions  $x(0) = x_0$ ,  $x'(0) = v_0$ . Calculate  $\langle x(t) \rangle_P$  and  $\langle (x - \langle x(t) \rangle_P)^2 \rangle_P$  where  $\langle f(x) \rangle_P = \int_{-\infty}^{\infty} f(x) W(x, t; x_0, v_0)$ .

b) Calculate the first 10 terms of the series of  $(1 + z/n)^n$  around  $n = \infty$ .

c) To improve the well-known formula  $\lim_{n \rightarrow \infty} (1 + 1/n)^n = e$ , we write [153★]

$$e = \left(1 + \frac{1}{n}\right)^{n + \sum_{k=0}^{\infty} \alpha_k n^{-k}}.$$

Calculate the first 100 of the  $\alpha_k$ . How precise is the approximation for  $n = 1$ ? Find the optimal  $\alpha_0$ ,  $\alpha_1$ ,  $\beta_2$ , and  $\beta_3$  in the following formula:

$$e = \lim_{n \rightarrow \infty} \left(1 + \frac{1}{n} + \frac{\beta_2}{n^2} + \frac{\beta_3}{n^3}\right)^{n + \alpha_0 + \frac{\alpha_1}{n}}.$$

d) The  $q$ -logarithm  $\ln_q(x)$  can be defined through  $\ln_q(x) = (x^{1-q} - 1)/(1 - q)$  [1334★] and fulfills the following identity for positive  $q$  and  $x_i$  [1888★]

$$\ln_q\left(\prod_{k=1}^n x_k\right) = \sum_{k=0}^n (1 - q)^{k-1} \left(\sum_{l_1=1}^n \sum_{l_2=l_1+1}^n \cdots \sum_{l_k=l_{k-1}+1}^n \prod_{j=1}^k \ln_q(x_{l_j})\right).$$

Verify this identity for  $2 \leq n \leq 10$  by explicit calculation of the left and right sides.

**20.<sup>L3</sup>  $S_{mn}$ , Symmetric Determinant, Fermat Test**

Implement an efficient computation for [1376★], [1611★], [968★], [188★]

$$S_{mn} = \Psi(mn + 1) - \frac{\int_0^\infty dq_1 \int_0^\infty dq_2 \cdots \int_0^\infty dq_m Q_{mn}(q_1, q_2, \dots, q_m)}{m n \int_0^\infty dq_1 \int_0^\infty dq_2 \cdots \int_0^\infty dq_m P_{mn}(q_1, q_2, \dots, q_m)}, \quad m \leq n$$

$$Q_{mn}(q_1, q_2, \dots, q_m) = \prod_{\substack{i,j=1 \\ i < j}}^m (q_i - q_j)^2 \prod_{k=1}^m e^{-q_k} q_k^{n-m}$$

$$P_{mn}(q_1, q_2, \dots, q_m) = Q_{mn}(q_1, q_2, \dots, q_m) \sum_{k=1}^m q_k \ln(q_k).$$

where  $\Psi(z)$  is the Digamma function. Compute the results for  $S_{ij}$ ,  $1 \leq i, j \leq 4$ . Can one compute  $S_{55}$  by brute force?

**b)** Let the symmetrized determinant of a matrix  $\mathbf{X}$  of dimension  $n \times n$  and elements  $x_{ij}$  be defined as [127★]

$$\text{sdet } \mathbf{X} = \frac{1}{n!} \sum_{\sigma \in S_n} \sum_{\tau \in S_n} \text{signature}(\sigma) \text{signature}(\tau) x_{\sigma(1)\tau(1)} \cdots x_{\sigma(n)\tau(n)}.$$

The summations run over all elements of the permutations  $S_n$  of  $\{1, 2, \dots, n\}$ .

Does there exist a  $4 \times 4$  matrix  $\mathbf{X}$  with elements

$$x_{ij} = c_{ij}^{(a)} a + c_{ij}^{(b)} b + c_{ij}^{(c)} c + c_{ij}^{(e)} e$$

where the  $c_{ij}^{(.)}$  are  $\pm 1$  or 0 and  $a, b, c$ , and  $e$  are noncommuting quantities with the multiplication table

$a$	$b$	$c$	$e$
$a$	$e$	$c$	$b$
$b$	$c$	$e$	$a$
$c$	$b$	$a$	$e$
$e$	$a$	$b$	$c$

such that  $\text{sdet } \mathbf{X} = a + b + c + e$ ?

**b)** Show that the following expression  $R$  (from [1147★] and <http://www.bway.net/~lewis/fermat/FerTest1>) vanishes identically. Use at least three different methods to show that  $R = 0$ . Try to minimize memory usage.

$$\begin{aligned} R = & q_2^2 q_3^2 (l_1 - 1)(l_2 - 1)(g^2 - n_{1,1} n_{2,2}) + q_3^2 l_1 l_2 (g^2 + n_{1,1} + n_{2,2} - n_{1,1} n_{2,2} - 1) + \\ & q_2^2 q_3^2 (g^2 l_1 + g^2 l_2 - 2 g^2 l_1 l_2 + l_2 n_{1,1} - l_1 l_2 n_{1,1} + l_1 n_{2,2} - l_1 l_2 n_{2,2} - l_1 n_{1,1} n_{2,2} - l_2 n_{1,1} n_{2,2} + 2 l_1 l_2 n_{1,1} n_{2,2}) - \\ & q_3 q_4 (g^2 + n_{1,1} + n_{2,2} - n_{1,1} n_{2,2} - 1)(l_2 p_{1,1} + l_1 p_{2,2}) - \\ & q_2^2 q_3 (g^2 - n_{1,1} n_{2,2})(2 - l_1 - l_2 - p_{1,1} + l_2 p_{1,1} - p_{2,2} + l_1 p_{2,2}) + \\ & q_1 q_2 q_3 q_4 (l_1 - 1)(l_2 - 1)(n_{2,2} p_{1,1} - g p_{1,2} - g p_{2,1} + n_{1,1} p_{2,2}) + \\ & q_1 q_3 l_1 l_2 (2 - n_{1,1} - n_{2,2} - p_{1,1} + n_{2,2} p_{1,1} - g p_{1,2} - g p_{2,1} - p_{2,2} + n_{1,1} p_{2,2}) + \\ & q_1 q_3 q_4 (-l_2 p_{1,1} + l_1 l_2 p_{1,1} + l_2 n_{2,2} p_{1,1} - l_1 l_2 n_{2,2} p_{1,1} - g l_2 p_{1,2} + \\ & \quad g l_1 l_2 p_{1,2} - g l_1 p_{2,1} + g l_1 l_2 p_{2,1} - l_1 p_{2,2} + l_1 l_2 p_{2,2} + l_1 n_{1,1} p_{2,2} - l_1 l_2 n_{1,1} p_{2,2}) + \\ & q_1 q_2 q_3 (-l_2 n_{1,1} + l_1 l_2 n_{1,1} - l_1 n_{2,2} + l_1 l_2 n_{2,2} + l_1 n_{2,2} p_{1,1} - l_1 l_2 n_{2,2} p_{1,1} - g l_1 p_{1,2} + \\ & \quad g l_1 l_2 p_{1,2} - g l_2 p_{2,1} + g l_1 l_2 p_{2,1} + l_2 n_{1,1} p_{2,2} - l_1 l_2 n_{1,1} p_{2,2}) + \\ & q_2 q_3 (-g^2 l_1 - g^2 l_2 - l_2 n_{1,1} - l_1 n_{2,2} + l_1 n_{1,1} n_{2,2} + l_2 n_{1,1} n_{2,2} + g^2 l_2 p_{1,1} + l_2 n_{1,1} p_{1,1} - \end{aligned}$$

$$\begin{aligned}
& l_2 n_{1,1} n_{2,2} p_{1,1} + g l_1 p_{1,2} + g l_2 p_{2,1} + g^2 l_1 p_{2,2} + l_1 n_{2,2} p_{2,2} - l_1 n_{1,1} n_{2,2} p_{2,2}) + \\
& q_2 q_3 q_4 (-g^2 p_{1,1} + g^2 l_2 p_{1,1} - n_{2,2} p_{1,1} + l_2 n_{2,2} p_{1,1} + n_{1,1} n_{2,2} p_{1,1} - l_2 n_{1,1} n_{2,2} p_{1,1} + g p_{1,2} - g l_1 p_{1,2} + \\
& g p_{2,1} - g l_2 p_{2,1} - g^2 p_{2,2} + g^2 l_1 p_{2,2} - n_{1,1} p_{2,2} + l_1 n_{1,1} p_{2,2} + n_{1,1} n_{2,2} p_{2,2} - l_1 n_{1,1} n_{2,2} p_{2,2}) + \\
& q_1^2 q_4^2 (l_1 - 1)(l_2 - 1)(p_{1,2} p_{2,1} - p_{1,1} p_{2,2}) - q_1 q_4^2 (2 - l_1 - l_2 - n_{1,1} + l_2 n_{1,1} - n_{2,2} + l_1 n_{2,2}) \\
& (p_{1,2} p_{2,1} - p_{1,1} p_{2,2}) - q_4^2 (g^2 + n_{1,1} + n_{2,2} - n_{1,1} n_{2,2} - 1)(p_{1,2} p_{2,1} - p_{1,1} p_{2,2}) - \\
& q_1^2 l_1 l_2 (1 - p_{1,1} - p_{1,2} p_{2,1} - p_{2,2} + p_{1,1} p_{2,2}) + q_1 q_2 (l_2 n_{1,1} + l_1 n_{2,2})(1 - p_{1,1} - p_{1,2} p_{2,1} - p_{2,2} + p_{1,1} p_{2,2}) + \\
& q_2^2 (g^2 - n_{1,1} n_{2,2})(1 - p_{1,1} - p_{1,2} p_{2,1} - p_{2,2} + p_{1,1} p_{2,2}) + \\
& q_1^2 q_4 (l_2 p_{1,1} - l_1 l_2 p_{1,1} + l_1 p_{1,2} p_{2,1} + l_2 p_{1,2} p_{2,1} - 2 l_1 l_2 p_{1,2} p_{2,1} + \\
& l_1 p_{1,2} p_{2,2} - l_1 l_2 p_{2,2} - l_1 p_{1,1} p_{2,2} - l_2 p_{1,1} p_{2,2} + 2 l_1 l_2 p_{1,1} p_{2,2}) + \\
& q_1 q_4 (-l_2 p_{1,1} + l_2 n_{1,1} p_{1,1} + g l_2 p_{1,2} + g l_1 p_{2,1} - l_1 p_{1,2} p_{2,1} - l_2 p_{1,2} p_{2,1} + l_2 n_{1,1} p_{1,2} p_{2,1} + l_1 n_{2,2} p_{1,2} p_{2,1} - \\
& l_1 p_{2,2} + l_1 n_{2,2} p_{2,2} + l_1 p_{1,1} p_{2,2} + l_2 p_{1,1} p_{2,2} - l_2 n_{1,1} p_{1,1} p_{2,2} - l_1 n_{2,2} p_{1,1} p_{2,2}) + q_1 q_2 q_4 \\
& (-n_{2,2} p_{1,1} + l_1 n_{2,2} p_{1,1} + g p_{1,2} - g l_2 p_{1,2} + g p_{2,1} - g l_1 p_{2,1} - n_{1,1} p_{1,2} p_{2,1} + l_2 n_{1,1} p_{1,2} p_{2,1} - n_{2,2} p_{1,2} p_{2,1} + \\
& l_1 n_{2,2} p_{1,2} p_{2,1} - n_{1,1} p_{2,2} + l_2 n_{1,1} p_{2,2} + n_{1,1} p_{1,1} p_{2,2} - l_2 n_{1,1} p_{1,1} p_{2,2} + n_{2,2} p_{1,1} p_{2,2} - l_1 n_{2,2} p_{1,1} p_{2,2}) + \\
& q_2 q_4 (g^2 p_{1,1} + n_{2,2} p_{1,1} - n_{1,1} n_{2,2} p_{1,1} - g p_{1,2} - g p_{2,1} + 2 g^2 p_{1,2} p_{2,1} + n_{1,1} p_{1,2} p_{2,1} + \\
& n_{2,2} p_{1,2} p_{2,1} - 2 n_{1,1} n_{2,2} p_{1,2} p_{2,1} + g^2 p_{2,2} + n_{1,1} p_{2,2} - n_{1,1} n_{2,2} p_{2,2} - \\
& 2 g^2 p_{1,1} p_{2,2} - n_{1,1} p_{1,1} p_{2,2} - n_{2,2} p_{1,1} p_{2,2} + 2 n_{1,1} n_{2,2} p_{1,1} p_{2,2}).
\end{aligned}$$

The  $q_i$  in the last polynomial are given by the following rational functions:

$$q_1 = -\frac{c_2 c_6}{c_3 c_5}, \quad q_2 = \frac{c_2 c_4}{c_1 c_5}, \quad q_3 = \frac{c_2 c_9}{c_3 c_8}, \quad q_4 = \frac{c_2 c_7}{c_1 c_8},$$

$$\begin{aligned}
c_1 &= (l_1 - 1) a_{1,2} a_{2,1} - (l_2 - 1) a_{2,2} \\
c_2 &= l_1 a_{1,2} (1 + a_{2,1}) - l_2 (a_{1,2} + a_{2,2}) \\
c_3 &= l_1 (1 + a_{2,1}) a_{2,2} + l_2 ((l_1 - 1) a_{1,2} a_{2,1} - (l_1 + a_{2,1}) a_{2,2}) \\
c_4 &= -a_{2,1} (g - a_{1,2} (n_{1,1} - 1)) + a_{2,2} (1 + g a_{1,2} - n_{2,2}) \\
c_5 &= -g + g a_{1,2}^2 - g a_{2,1} + a_{1,2} (g a_{2,2} + (1 + a_{2,1}) n_{1,1} - n_{2,2}) - a_{2,2} n_{2,2} \\
c_6 &= g a_{2,1}^2 - a_{2,2} (g^2 + g (a_{1,2} + a_{2,2}) - n_{1,1} (n_{2,2} - 1)) + \\
& a_{2,1} (g + a_{2,2} (n_{2,2} - n_{1,1}) + a_{1,2} (g^2 - (n_{1,1} - 1) n_{2,2})) \\
c_7 &= -a_{2,1} p_{1,2} + a_{1,2} (a_{2,1} (p_{1,1} - 1) + a_{2,2} p_{2,1}) - a_{2,2} (-1 + p_{2,2}) \\
c_8 &= -(1 + a_{2,1}) p_{1,2} + a_{1,2}^2 p_{2,1} + a_{1,2} ((1 + a_{2,1}) p_{1,1} + a_{2,2} p_{2,1} - p_{2,2}) - a_{2,2} p_{2,2} \\
c_9 &= a_{2,2}^2 p_{2,1} + a_{2,1} (-p_{1,2} (1 + a_{2,1} + a_{1,2} p_{2,1}) + a_{1,2} (p_{1,1} - 1) p_{2,2}) + \\
& a_{2,2} ((1 + a_{2,1}) p_{1,1} + (a_{1,2} + p_{1,2}) p_{2,1} - (a_{2,1} + p_{1,1}) p_{2,2})
\end{aligned}$$

### 21.<sup>L3</sup> WKB Approximations of Higher Order, GHZ State, Entropic Uncertainty Relation

a) This problem is meant for those who are already familiar with WKB approximations in quantum mechanics [1612★], [897★]—an approximate solution for the eigenvalue of the 1D Schrödinger equation. (In the following,  $m = 1$  and  $\hbar = h/(2\pi)$  explicitly stand for the derivation of the relevant equations determined by a “small” parameter, the so-called WKB approximation.)

$$\left( -\frac{\hbar^2}{2} \frac{d^2}{dx^2} + V(x) - E \right) \Psi(x) = 0$$

We restrict ourselves here to the case in which the potential has just one minimum. Assuming a solution of the form

$$\Psi(x) = \exp\left(i \frac{1}{\hbar} \int^x S(x) dx\right)$$

$$S(x) = \sum_{k=0}^{\infty} \left(\frac{\hbar}{i}\right)^k S_k(x)$$

for the Schrödinger equation, we get the following recurrence formula for  $S_n(x)$  [1126★], [808★], [1510★], [732★], [496★]:

$$S_0(x) = \sqrt{E - V(x)}$$

$$S'_{n-1}(x) = \sum_{m=0}^n S_{n-m}(x) S_m(x).$$

Now, interpreting  $x$  as a complex variable and  $V(x)$  as a complex function, we are led to the following condition for the eigenvalue  $E$  [1754★]:

$$\oint S_0(x) dx + \sum_{k=1}^{\infty} \left(\frac{\hbar}{i}\right)^k \oint S_k(x) dx = \left(n + \frac{1}{2}\right) h$$

Thus,  $E_j$  ( $j = 0, 1, \dots$ ) is an eigenvalue for the above differential equation if and only if this equation is satisfied. The  $x$ -integrals are taken along a path in the complex  $x$ -plane that contains both of the classical turning points  $x_1$  and  $x_2$ . Both  $x_1$  and  $x_2$  are solutions of the equation  $V(x) = E$ .

Frequently, the potential  $V(x)$  is given only for real numbers  $x$  (perhaps from a numerical calculation). Then, the above integral formula is of little use. Even if we put the integration path on the real axis, for  $n > 1$ , in general,  $S_n(x)$  has a nonintegrable singularity. Moreover, the integrands that arise can be greatly simplified by integration by parts.

One way out of these difficulties is to use integration by parts with respect to  $x$ , and to reduce the strongly singular integrands to integrable integrands using integration by parts over  $E$  [659★], [1338★]. (For details, see [1088★], [1087★], [541★], [51★], [1277★], [144★], [72★], [16★], [1356★], [1872★], [162★], [1016★], [1017★], [646★], [1508★], [348★], [336★], [1018★], [1019★], [44★], [549★], [625★], [599★], [274★], [1892★], [1206★], and [1812★].)

Implement the computation of these reduced forms of the integrals over the  $S_n(x)$  for  $n = 1$  to 10. To this end, first find  $S_n(x)$ , and then integrate the parts containing  $V'(x)$  as often as possible by parts. Write the resulting expressions over all denominators that appear, and integrate the terms so obtained as often as possible by parts, without increasing the maximum singularity in the current denominator. Finally, integrate the expressions thus obtained by parts with respect to  $E$ , and write the results in an appropriate form.

For  $V(x) = x^4$  [1509★], [1813★], calculate the correction terms explicitly. Compare for the value  $\hbar=1/10$  and  $\hbar=1/100$  the convergence behavior of  $n = 3$  and  $n = 100$ .

**b)** This is another problem for readers who are with quantum mechanics. For the three-particle Greenberger–Horne–Zeilinger state [1259★], [454★], [141★], [1165★], [1914★], [290★], [11★], [792★], and [1735★]  $|\Psi\rangle = (|\uparrow\rangle_1 |\uparrow\rangle_2 |\uparrow\rangle_3 - |\downarrow\rangle_1 |\downarrow\rangle_2 |\downarrow\rangle_3) / 2^{1/2}$  find the most general observable  $\hat{E}_{\pm} = (\vec{n}_1 \cdot \vec{\sigma})_1 \otimes \mathbf{1} \otimes \mathbf{1} \otimes (\vec{n}_2 \cdot \vec{\sigma})_2 \otimes \mathbf{1} \otimes \mathbf{1} \otimes (\vec{n}_3 \cdot \vec{\sigma})_3$  (with normalized  $|\vec{n}_k| = 1$ ) such that  $\hat{E}_{\pm} |\Psi\rangle = \pm 1 |\Psi\rangle$ . ( $\vec{\sigma}$  is the vector of the three Pauli matrices.)

**c)** And one more exercise for the friends of quantum mechanics: Does there exist a pure (entangled) state of four (different) spin 1/2 particles [1550★], [323★], [1666★], [570★], [852★], [547★], [342★], [1399★] such that all two-particle reduced density matrices are multiples of the identity?

**d)** The entropic uncertainty relation is  $\delta x \delta p \geq \pi e \hbar$  [1566★], [888★], [1191★]. Here the  $\delta a$  is the exponential of the differential entropy  $\delta a = \exp\left(-\int_{-\infty}^{\infty} w(a) \ln(w(a)) da\right)$  of the normalized to  $\int_{-\infty}^{\infty} w(a) da = 1$  probability density  $p(a)$  [888★]. For the

simplest case of a 1D scattering on a slit of length  $2L$  with the position probability density  $w(x) = \theta(L+x)\theta(L-x)(2L)^{-1/2}$ , calculate  $\delta p$  whose probability density is  $w(p) = \left| \int_{-\infty}^{\infty} \exp(ipx) w(x)^{1/2} dx \right|^2$  [1566★].

## 22.<sup>L3</sup> QES Condition, Integral of Rational Function, Integrals of Roots, Triangle Roots

a) Calculate the symbolic value of  $\alpha$  such that  $i = \int_{-x_0}^{x_0} \sqrt{\alpha - x^6 + 4x^2} dx$ , where  $x_0$  is the real positive root of a  $\alpha - x^6 + 4x^2 = 0$  takes the value  $i = 2\pi$ . (The answer for  $\alpha$  is a “nice” algebraic number [147★], [1769★].)

b) Calculate the value of the integral  $\int_{-\infty}^{\infty} (z^8 + 7z^6 + 5z^4 + 3z^2 + 1)^{-4} dz$ . Express the result in a nice form [212★], [1295★].

c) Calculate the following integral ( $x > 1$ ) [1606★]:

$$\lim_{\gamma \rightarrow 0} \int_1^{\infty} \frac{z^\gamma - 1}{\gamma z^2} (1 + x(z^\gamma - 1))^{-\frac{1}{\gamma} - 1} dz.$$

d) Let  $\mathcal{R}_k(\xi, a_0 + a_1 \xi + \dots + a_n \xi^n)$  stand for the root that is represented by the Root-object `Root` [ $a_0 + a_1 \# + \dots + a_n \#^n$ ,  $k$ ]. Calculate the following integrals symbolically (express the results using Root-objects):

$$\int \ln(x^2) \mathcal{R}_1(\xi, -x - x\xi + \xi^6) dx$$

$$\int \exp(\mathcal{R}_3(\xi, -x - \xi^2 + \xi^7)) \ln(\mathcal{R}_3(\xi, -x - \xi^2 + \xi^7)) \mathcal{R}_3(\xi, -x - \xi^2 + \xi^7) dx$$

$$\int \sqrt{\frac{\mathcal{R}_2(\xi, -x - \xi + \xi^3)}{\mathcal{R}_3(\xi, -x - \xi + \xi^3)}} dx$$

$$\int \sqrt[3]{\frac{\mathcal{R}_2(\xi, -x - x\xi + \xi^3)}{\mathcal{R}_3(\xi, -x - x\xi + \xi^3)}} dx$$

$$\int_0^1 \frac{\mathcal{R}_2(\xi, -x - \xi + \xi^3)}{\mathcal{R}_2(\xi, x - \xi + \xi^3) - 1} dx$$

$$\int_1^{\infty} \left( \frac{1}{\mathcal{R}_1(\xi, -x + \xi + \xi^5)} - \frac{1}{5x} - \frac{1}{\sqrt[3]{x}} \right) dx$$

e) Under which conditions on  $a_1, a_2, a_3$  can the three roots of the cubic  $x^3 + a_1 x^2 + a_2 x + a_3 = 0$  be interpreted as the side length of a nondegenerate triangle [1349★]? Visualize the volume in  $a_1, a_2, a_3$ -space for which this happens. For random  $a_1, a_2, a_3$  from the interval  $[-1, 1]$ , what is the probability that the roots are the side length of a nondegenerate triangle?

## 23.<sup>L2</sup> Riemann Surface of Cubic

Visualize the Riemann surface of  $x(a)$ , where  $x = x(a)$  is implicitly given by  $x^3 + x^2 + ax - 1/2 = 0$ . Do not use `ContourPlot3D`.

## 24.<sup>L2</sup> Celestial Mechanics, Lagrange Points

a) For the so-called Kepler equation (see [1343★], [1714★], [1532★], [787★], [1247★], [305★], [346★], and [392★])  $L = M + \epsilon \sin(L)$  find a series solution for small  $\epsilon$  in the form



$$L \approx M + \sum_{i=1}^n \left( \sum_{j=i}^{n \text{ or } n-1} a_{ij} \epsilon^j \right) \sin(i M)$$

with  $n$  around 10.

**b)** Find a short time-series solution (power series in  $t$  up to order 10, for example) for the equation of motion for a body in a spherical symmetric gravitational field (to avoid unnecessary constants, appropriate units are chosen)

$$\mathbf{r}''(t) = \frac{\mathbf{r}(t)}{r(t)^3}$$

with the initial conditions  $\mathbf{r}(0) = \mathbf{r}_0$ ,  $\mathbf{r}'(0) = \mathbf{v}_0$ . Here,  $\mathbf{r}(t)$  is the time-dependent position vector of the body and  $r(t) = |\mathbf{r}(t)|$ . To shorten the result, introduce the abbreviations

$$s = \frac{\mathbf{r}_0 \cdot \mathbf{v}_0}{r_0^2} \quad w = \frac{\mathbf{v}_0 \cdot \mathbf{v}_0}{r_0^2} \quad u = \frac{1}{r_0^3}$$

(Do not use explicit lists as vectors, first because this is explicitly dependent on the dimension, and second because it slows down the calculation considerably. It is better to implement an abstract vector type for  $\mathbf{r}(t)$  and define appropriate rules for it.)

**c)** The Lagrange points  $\{x(\mu), y(\mu)\}$  of the restricted three-body problem are the solutions of the following system of equations [435★], [1432★], [1771★], [807★], [1444★], [750★], [139★]:

$$-\frac{\partial V(x, y)}{\partial x} = -\frac{\partial V(x, y)}{\partial y} = 0.$$

The potential  $V(x, y)$  is given by the following expression:

$$V(x, y) = -\frac{1}{2}(x^2 + y^2) - \frac{1-\mu}{r_1} - \frac{\mu}{r_2}$$

$$r_1 = \sqrt{(x-x_1)^2 + y^2}$$

$$r_2 = \sqrt{(x-x_2)^2 + y^2}$$

$$x_1 = -\mu$$

$$x_2 = 1 - \mu$$

Calculate explicit symbolic solutions for the Lagrange points. For the parameter value  $\mu = \frac{1}{10}$ , calculate all real solutions (do not do this by a direct call to `Solve`).

## 25.<sup>L2</sup> Algebraic Lissajous Curves, Light Ray Reflection Inside a Closed Region

**a)** Derive an implicit representation  $f(x, y)$  of the Lissajous curves  $\{x(t), y(t)\} = \{\cos(t), \sin(2t)\}$ ,  $\{x(t), y(t)\} = \{\cos(3t), \sin(2t)\}$  and some higher-order Lissajous curves.

**b)** Describe the region that is given implicitly by

$$(9x^2 - 24x^4 + 16x^6 - 4y^2 + 4y^4)^2 - \frac{1}{2} < 0$$

explicitly in terms of a conjunction of 2D sets. Each set described by a pair of inequalities of the form

$$x_l \leq x \leq x_u, \quad y_l(x) \leq y \leq y_u(x)$$

Use this description to generate a picture of this region (the name *lissa* stems from the fact that  $9x^2 - 24x^4 + 16x^6 - 4y^2 + 4y^4$  is the implicit description of a Lissajous curve). (Do not use `CylindricalDecomposition`, `Reduce` or similar functions.)

c) Derive the implicit representation  $f(x, y)$  of the evolute of the Lissajous curves  $\{x(t), y(t)\} = \{\cos(t), \sin(2t)\}$ . For an implicitly defined curve  $g(x, y)$ , the points  $\{\xi, \eta\}$  of the evolute are given by

$$\xi = x - \frac{g_x(g_x^2 + g_y^2)}{g_y^2 g_{xx} - 2g_x g_y g_{xy} + g_x^2 g_{yy}} \quad \eta = y - \frac{g_y(g_x^2 + g_y^2)}{g_y^2 g_{xx} - 2g_x g_y g_{xy} + g_x^2 g_{yy}}$$

where  $g_x = \partial g(x, y) / \partial x$ ,  $g_y = \partial g(x, y) / \partial y$ , and so on.

d) Make an animation showing how the orthopodic locus [858★], [1881★] of the Lissajous curves  $\{x(t), y(t)\} = \{\cos(t), \sin(2t)\}$  is generated. The orthopodic locus of a curve is the set of all points where two tangents on the given point intersect perpendicularly. Derive the implicit representation  $f(x, y)$  of the orthopodic locus of the Lissajous curves under consideration. Do not solve nonpolynomial equations numerically here.

e) Calculate the implicit equation of the cissoid [858★] of the Lissajous curves  $\{x(t), y(t)\} = \{\cos(t), \sin(2t)\}$ . The cissoid of a curve and a given point  $P$  is the set of all points that lie on a line through  $P$  and are at the same time the midpoint of the line segment formed by two points of the given curve. For  $P = \{1/2, 1/2\}$ , make a picture of the implicit representation and compare it with a straightforward calculation of the cissoid.

f) Make a picture with the implicit equation of the  $\{\cos(3\varphi) - \sin(\varphi)/5, \sin(2\varphi) + \cos(\varphi)/3\}$ ,  $0 \leq \varphi \leq 2\pi$  written along the curve itself.

g) Follow a light ray that is ideally reflected multiple times inside the two-dimensional region defined by  $x^4 + y^4 - 2x^3 + 2y + 2x - 1 \leq 0$  (a billiard problem [964★]). Determine some (and if possible all) stationary light rays.

h) The hedgehog of a function  $h(t)$  is the envelope of the family of lines  $x \cos(t) + y \sin(t) = h(t)$  [1223★]. Calculate and visualize the hedgehog of  $h(t) = -\cos(t) + 2 \cos(6t)$ .

i) Make an animation of the following function inside the region  $x^4 + y^4 < 1$  as  $k$  varies from 0 to 150:

$$I_k(x, y) = \int_0^L \exp(ik d(\{x, y\}, \{\xi(s), \eta(s)\})) \delta(g(\{x, y\}, \{\xi(s), \eta(s)\})) ds.$$

Here  $s$  is the arclength of the curve  $C$  implicitly described through  $x^4 + y^4 = 1$ ,  $L$  its length,  $g(\{x, y\}, \{\xi(s), \eta(s)\}) = a(s)y + b(s)x + c(s)$  is the implicit equation for the lines through the point  $\{x, y\}$  that are perpendicular to  $C$  at  $\{\xi(s), \eta(s)\}$ , and  $d(\{x, y\}, \{\xi(s), \eta(s)\})$  is the distance of the point  $\{x, y\}$  to the point  $\{\xi(s), \eta(s)\}$ . For some selected  $k$ , compare the resulting graphics with a corresponding graphic of

## 26.<sup>L2</sup> Change of Variables in a Differential Equation, Functional Equation

a) Given the following initial value problem [626★]:

$$\begin{aligned} y''(x) &= x^3 + y(x)^3 + y'(x)^3 \\ y(0) &= 0 \\ y'(0) &= 0 \end{aligned}$$

Derive a new differential equation for  $u(x_1)$  when using the following change of variables on the above differential equation:

$$\begin{aligned} x_1 &= y'(x) \\ u(x_1) &= y(x) \end{aligned}$$

Calculate 10 terms of the series of  $u(x_1)$  around  $x_1$  and compare the quality of the series solution with a numerical solution.

b) Let the function  $f_q(z)$  be defined through the functional equation  $f_q(qz) = (q f_q(z)^2 - q + 2)/2$  [768★], [708★], [1736★], [416★], [251★], [1193★], [1194★]. Make an animation of  $f_{1.6 \exp(i\varphi)}(z)$  as a function of real  $\varphi$ .

## 27.<sup>L2</sup> Discriminant Surface, Multivalued Surface, 27 Lines on the Clebsch Surface

a) Make a picture of the surface [1792★], [1868★], [1003★] defined implicitly by

$$256z^3 + 128x^2z^2 + 16x^4z - 144xz^2y^2 - 4x^3y^2 + 27y^4 = 0$$

in the  $x, y$ -region  $(-1, 2) \times (-3/2, 3/2)$  and in the corresponding  $z$ -region. Using `ContourPlot3D` will not show all details with sufficient quality.

b) Make a picture of the following implicitly defined surface

$$\sin(x)\cos(y) + \sin(y)\cos(z) + \sin(z)\cos(x) = 0$$

in the cube  $0 \leq x \leq 2\pi, 0 \leq y \leq 2\pi, 0 \leq z \leq 2\pi$ . Do not use `ContourPlot3D` for generating the picture.

c) The Clebsch surface (see also Exercise 7 of Chapter 1 of the Numerics volume [1752★]), defined by the implicit equation

$$32 - 216x^2 + 648x^2y - 216y^2 - 216y^3 - 150z + 216x^2z + 216y^2z + 231z^2 - 113z^3 = 0$$

has the remarkable property that 27 straight lines lie on it [555★], [1512★], [838★], [1043★], [644★], [1607★], [1602★], [28★], [863★]. Calculate these 27 lines explicitly. Visualize these lines that lie on the surface.

d) Calculate the implicit representations of “generalized” Clebsch surfaces, which, instead of a threefold rotation symmetry, have an  $n$ -fold rotation symmetry ( $n = 4, 5, 6, \dots$ ) and has a similar shape. Visualize some of them.

## 28.<sup>L2</sup> 28 Bitangents on a Real Plane Quartic, Curve Intersections, Pentaellipse

a) In [560★], the following implicit equation for a plane quartic with 28 real bitangents is given. (A bitangent is a line that is tangent to two points, including the degenerate case in which these two points coincide) and to a curve at the same time.

$$x^4 + y^4 - 6(x^2 + y^2) + 10 = 0$$

Calculate the explicit form of the bitangents, and make a picture that illustrates that these lines are bitangents.

b) Consider the parametric curve  $\{\operatorname{Re}(z(\varphi)), \operatorname{Im}(z(\varphi))\}$  where  $z(\varphi)$  is implicitly defined by  $2z(\varphi)^6 = q(\varphi) + q(\varphi)^3$  and  $q = R \exp(i\varphi)$ ,  $R = 9/10$ . Find exact values for the points where the curve self-intersects.

c) An ellipse can be defined as the set of points whose sum of distances from two points is a constant. A natural generalization of this definition is the set of points whose sum of distances from  $n$  points is a constant  $c$  [618★], [1610★], [1418★]. For the case of  $n = 5$  and the five points being the vertices of a regular pentagon, derive a polynomial  $p_c(x, y)$  (with integer coefficients) such that  $p_c(x, y) = 0$  contains the pentaellipse. Visualize  $p_c(x, y) = 0$ .

## 29.<sup>L2</sup> Maxwell's Equations Are Galilei Invariant, X-Waves, Fields in a Moving Media, Thomas Precession, Retarded Potential Expansion

a) Show that the vacuum Maxwell equations [938★] (the fields  $\vec{E}, \vec{H}$  are functions of the coordinates  $x, y, z$ .)

$$\begin{aligned}\frac{\partial \vec{E}}{\partial t} &= \text{curl } \vec{H} \\ \frac{\partial \vec{H}}{\partial t} &= -\text{curl } \vec{E} \\ \text{div } \vec{E} &= 0 \\ \text{div } \vec{H} &= 0\end{aligned}$$

are invariant under the Galilei transformation

$$\begin{aligned}\vec{r}' &= \vec{r} + \vec{v} t \\ t' &= t\end{aligned}$$

if the fields are transformed in the following way:

$$\begin{aligned}\vec{E}' &= \vec{E} - \vec{v} \times \vec{H} - \left( \vec{v} \cdot \vec{r} + \frac{t}{2} \vec{v} \cdot \vec{v} \right) \text{rot } \vec{H} + \frac{1}{2} \left( v^2 \vec{E} - \vec{v} \vec{v} \cdot \vec{E} + \vec{r} \cdot \vec{v} (\nabla \cdot \vec{v} \vec{E} - 2 \vec{v} \times \text{rot } \vec{E}) + (\vec{r} \cdot \vec{v})^2 \Delta \vec{E} \right) + O(v^3) \\ \vec{H}' &= \vec{H} + \vec{v} \times \vec{E} - \left( \vec{v} \cdot \vec{r} + \frac{t}{2} \vec{v} \cdot \vec{v} \right) \text{rot } \vec{E} + \frac{1}{2} \left( v^2 \vec{H} - \vec{v} \vec{v} \cdot \vec{H} + \vec{r} \cdot \vec{v} (\nabla \cdot \vec{v} \vec{H} - 2 \vec{v} \times \text{rot } \vec{H}) + (\vec{r} \cdot \vec{v})^2 \Delta \vec{H} \right) + O(v^3) \\ v &= |\vec{v}|\end{aligned}$$

For the derivation of these formulae, see [684★] and [1075★]. (For related discussions see [1136★], [740★], [1076★].)

b) The relativistic relations between the electric and magnetic vacuum fields  $\mathcal{E}$ ,  $\mathcal{H}$  and the electric and magnetic fields in media  $\mathcal{D}$ ,  $\mathcal{B}$  [1511★] are given by [842★], [1915★], [1245★]

$$\begin{aligned}\mathcal{D} + \frac{1}{c} \mathbf{v} \times \mathcal{H} &= \varepsilon \left( \mathcal{E} + \frac{1}{c} \mathbf{v} \times \mathcal{B} \right) \\ \mathcal{B} - \frac{1}{c} \mathbf{v} \times \mathcal{E} &= \mu \left( \mathcal{H} - \frac{1}{c} \mathbf{v} \times \mathcal{D} \right)\end{aligned}$$

Here,  $\mathbf{v}$  is the velocity of the moving media,  $\varepsilon$  and  $\mu$  are the relative permittivity and permeability. Express the fields  $\mathcal{D}$ ,  $\mathcal{B}$  as a function of  $\mathcal{E}$ ,  $\mathcal{H}$  in compact vector form. (Do not guess the form; derive it.)

c) Show that  $\text{Re}(\varphi_v(\rho, z; t))$  where [1905★], [1615★], [167★]

$$\varphi_v(\rho, z; t) = \frac{z - vt + i\alpha}{\left( (z - vt + i\alpha)^2 + \left(1 - \frac{v^2}{c^2}\right) \rho^2 \right)^{3/2}}$$

is a solution of the 3D wave equation ( $\rho$ , and  $z$  are cylindrical coordinates,  $c$  is the group velocity,  $\alpha$  and  $v$  are arbitrary parameters). Visualize the solution for  $v \lesssim c$ .

d) Solve the following set of equations for  $\psi = \psi(\xi, \eta, \alpha)$ , eliminating the variables  $\rho$ , and  $\theta$  [355★].

$$e^{-\xi \sigma_3} e^{\eta (\sin(\alpha) \sigma_1 + \cos(\alpha) \sigma_3)} = e^{\rho (\sin(\theta) \sigma_1 + \cos(\theta) \sigma_3)} e^{i \psi \sigma_2}$$

Here  $e^{\text{matrix}}$  denotes the matrix exponential functions and the three  $\sigma_k$  are the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

$(\psi(\xi, \eta, \alpha))$  is the Thomas precession angle [415★], [1557★], [1766★], [158★], [1015★], [1765★], [1314★], [846★], [356★], [931★], [129★], [1489★] that arises from two successive Lorentz transformations in different directions as one Lorentz transformation and a rotation.)

e) Calculate the first few terms of the expansion in  $c^{-1}$  [463★], [760★], [1884★], [761★], [861★], [693★], [1814★], [1008★], [1815★], [181★], [224★], [798★], [1248★] of the Lienárd–Wiechert potential  $\varphi(\mathbf{r}, t)$

$$\varphi(\mathbf{r}, t) = \frac{e}{r(\tau) - \frac{1}{c} \mathbf{r}(\tau) \cdot \mathbf{v}(\tau)}$$

Here  $e$  is the electric charge,  $c$  is the speed of light,  $\mathbf{r}(\tau) = \mathbb{R} - \mathbb{R}_e(\tau)$ , where  $\mathbb{R}$  is the observation point and  $\mathbb{R}_e(\tau)$  the position of the charge. The scalar distance is  $r(\tau) = |\mathbf{r}(\tau)|$  and  $\mathbf{v}(\tau) = \partial \mathbb{R}_e(\tau) / \partial \tau$  is the velocity of the charge. The retarded time  $\tau$  is defined through  $t = \tau + r(\tau) / c$ .

f) Find a nontrivial “spherical”, standing wave-like solutions of the homogeneous Maxwell equations.

$$\begin{aligned} \operatorname{div} \mathcal{E}(\mathbf{r}, t) &= 0 \\ \operatorname{div} \mathcal{B}(\mathbf{r}, t) &= 0 \\ \frac{\partial \mathcal{E}(\mathbf{r}, t)}{\partial t} &= \operatorname{curl} \mathcal{B}(\mathbf{r}, t) \\ \frac{\partial \mathcal{B}(\mathbf{r}, t)}{\partial t} &= -\operatorname{curl} \mathcal{E}(\mathbf{r}, t) \end{aligned}$$

Here by “spherical” we mean a solution that does not depend on the azimuthal coordinate  $\varphi$ , but only on  $r$  and  $\vartheta$ . By “standing wave-like”, we mean  $\mathcal{E}(\mathbf{r}) \cdot \mathcal{B}(\mathbf{r}) = 0$ . For a wave-like solution, assume the time dependence of the form  $\mathcal{E}(\mathbf{r}) \sim \sin(t)$  and  $\mathcal{B}(\mathbf{r}) \sim \cos(t)$ . Use for the spatial part of the components  $e_a \in \{\mathcal{E}_r, \mathcal{E}_\vartheta, \mathcal{E}_\varphi, \mathcal{B}_r, \mathcal{B}_\vartheta, \mathcal{B}_\varphi\}$  of the fields in spherical coordinates  $\mathcal{E}(\mathbf{r}) = \mathcal{E}_r \mathbf{e}_r + \mathcal{E}_\vartheta \mathbf{e}_\vartheta + \mathcal{E}_\varphi \mathbf{e}_\varphi$ ,  $\mathcal{B}(\mathbf{r}) = \mathcal{B}_r \mathbf{e}_r + \mathcal{B}_\vartheta \mathbf{e}_\vartheta + \mathcal{B}_\varphi \mathbf{e}_\varphi$  an ansatz of the form [373★], [374★]

$$e_a \sim \sum_{\rho_r=-3}^1 \sum_{\rho_c, \rho_s=0}^1 \sum_{k,l=0}^o \sum_{\alpha_{c,k}, \alpha_{s,k}=0}^1 c_{\rho_r, \rho_c, \rho_s, k, l, \alpha_{c,k}, \alpha_{s,k}}^{(e,a)} r^{\rho_r} \cos(r)^{\rho_c} \sin(r)^{\rho_s} \cos(k \vartheta)^{\alpha_{c,k}} \sin(l \vartheta)^{\alpha_{s,l}}$$

for some (small integer)  $o$ . Here the  $c_{\rho_r, \rho_c, \rho_s, k, l, \alpha_{c,k}, \alpha_{s,k}}^{(e,a)}$  are constants independent of  $r$  and  $\vartheta$ . Visualize the motion of a charged particle in such fields.

### 30. L2 Asymptotic Series for $n!$ , $q$ -Series to $q$ -Product, $q$ -Binomial, gcd-Free Partitions

a) The series of  $n!$  is around  $n = \infty$  asymptotic. So to get the best numerical result from such a series in dependence of  $n$ , the series should be truncated in an  $n$ -dependent manner. Calculate after how many terms it is best to truncate the series for  $n = 1!, \dots, 15!$  (For a detailed exposition on the optimal truncation of divergent series, see [122★] and [492★].)

b) Ramanujan gave the following expansion for the factorial function for large  $n$  [159★], [46★]:

$$n! = \sqrt{\pi} \left(\frac{n}{e}\right)^n \left(8n^3 + 4n^2 + n + \frac{1}{30} + R(n)\right)^{1/6}$$

Assuming that  $R(n)$  is of the form  $\sum_{k=1}^{\infty} c_k n^{-k}$ , calculate the first few  $c_k$ . How many  $c_k$  are needed to calculate 100! to 100 correct digits?

c) Given a  $q$ -series  $\Sigma = 1 + \sum_{k=1}^n c_k q^k$ ,  $c_k \in \mathbb{Z}$ , write a one-liner `qSeriesToqProduct` that expresses the series  $\Sigma$  as a product

$$\Pi = \prod_{k=1}^m (1 - q^k)^{\alpha_k}, \alpha_k \in \mathbb{Z},$$

such that  $\Pi - \Sigma = O(q)^{n+1}$  [703★], [213★].

d) The  $q$ -binomial coefficients [605★], [97★], [1663★], [60★], [1070★], [143★], [1586★], [1105★], [1036★], [1549★], [258★]

$$\begin{bmatrix} n \\ k \end{bmatrix}_q = \frac{\prod_{j=1}^{n-k+1} (1 - q^j)}{\prod_{j=1}^k (1 - q^j)}$$

that are seemingly rational functions in  $q$ , are actually polynomials in  $q$ . For  $1 \leq k, n \leq 250$ , visualize the number of factors in the factored form of the  $q$ -binomial coefficient  $s$ . (The coefficient of  $q^k$  of  $\begin{bmatrix} m+n \\ n \end{bmatrix}_q$  is the number of partitions of  $k$  elements into at most  $n$  parts each part having at most  $m$  elements.)

e) A Taylor series  $c_0 + \sum_{j=1}^{\infty} c_j q^k$  is called multiplicative if  $c_{k \times l} = c_k c_l$  for all pairs  $k, l$ , such that  $\gcd(k, l) = 1$ . Products of the form

$$\frac{\prod_{j=1}^m \prod_{k=1}^{\infty} (1 - q^{\alpha_j k})^{\mu_j}}{\prod_{j=1}^n \prod_{k=1}^{\infty} (1 - q^{\beta_j k})^{\nu_j}}$$

where  $\sum_{j=1}^m \alpha_j \mu_j = \sum_{j=1}^n \beta_j \nu_j = s$  and the  $\alpha_j, \beta_j$  are all divisors of  $n = \max(\alpha_j, \beta_j)$  are sometimes multiplicative series [641★], [1472★]. Find all such type multiplicative series for  $1 \leq n, s \leq 24$ .

f) Given a set of distinct primes  $\{p_1, \dots, p_r\}$ , the number of partitions  $P_{p_1, \dots, p_k}(n)$  of a positive integer  $n$  into integers  $\{m_1, \dots, m_j\}$  (meaning  $\sum_{i=1}^j m_i = n$ ) such that  $\gcd(m_i, p_q) = 1, 1 \leq i \leq j, 1 \leq q \leq r$  is given by [1507★]

$$P_{p_1, \dots, p_k}(n) = [z^n] \left( \prod_{s=1}^{\infty} C_s(z^s)^{(-1)^{s-1}} \right)$$

where  $s = \prod_{q=1}^r p_q$  and  $C_s(z)$  is the  $s$ th cyclotomic polynomial (in *Mathematica* `Cyclotomic[s, z]`).

Use this formula to calculate  $P_{2,3,5,7,11}(111)$ . Compare the result with a direct calculation of the partitions themselves.

### 31.<sup>L2</sup> One ODE for the Kepler Problem, Euler Equations, $u(x) = \alpha \exp(\beta(z - z_0)^{-1/2})$ , Lattice Green's Function ODE

a) Construct one differential equation for the  $x$ -component  $x(t)$  of the radius vector of the 2D Kepler problem:

$$x''(t) = \frac{x(t)}{\sqrt{x(t)^2 + y(t)^2}}$$

$$y''(t) = \frac{y(t)}{\sqrt{x(t)^2 + y(t)^2}}$$

b) Construct one differential equation for the  $x(t)$  of the radius vector of equations of motion for a freely rotating body:

$$x'(t) = A y(t) z(t)$$

$$y'(t) = B x(t) z(t)$$

$$z'(t) = C x(t) y(t)$$

- c) Find a polynomial differential equation  $P(u(x), u'(x), u''(x), u'''(x)) = 0$  for the function  $u(x) = \alpha \exp(\beta / \sqrt{z - z_0})$  [1099★].
- d) Given the Darboux–Halphen system of differential equations [8★]

$$\begin{aligned}w'_1(z) &= w_1(z)(w_2(z) + w_3(z)) - w_2(z)w_3(z) \\w'_2(z) &= w_2(z)(w_1(z) + w_3(z)) - w_1(z)w_3(z) \\w'_3(z) &= w_3(z)(w_1(z) + w_2(z)) - w_1(z)w_2(z)\end{aligned}$$

find an (ordinary nonlinear) differential equation for  $W(z) = 2(w_1(z) + w_2(z) + w_3(z))$ .

- e) Derive  $x$ -free, polynomial differential equations for the two functions  $f(x) = \exp(\exp(\exp(e^x)))$  and  $g(x) = x^x$ .
- f) The following function  $G_\alpha(w)$  [1622★], [1298★], [1553★], [556★], [1002★], [966★], [967★] fulfills a linear homogeneous differential equation with respect to  $w$  with polynomial coefficients in  $\alpha$  and  $w$  [920★], [473★], [965★]:

$$G_\alpha(w) = \frac{1}{\pi^3} \int_0^\pi \int_0^\pi \int_0^\pi \frac{1}{w - (\cos(\theta_1) + \cos(\theta_2) + \alpha \cos(\theta_3))} d\theta_1 d\theta_2 d\theta_3$$

Use a series expansion in  $w$  to find such a differential equation.

### 32.<sup>L2</sup> Puzzles

- a) Can one find an example in which `DSolve[eqs, vars]` remains unsolved, but applying `ExpandAll[DSolve[eqs, vars]]` gives a result?

- b) What will be the result of the following inputs?

```
Integrate[Integrate[x^x, x]^3, Integrate[x^x, x]]
```

```
D[D[1[1], 1]^2, D[1[1], 1]]
```

```
Sum[Sum[k, {1, 4}]^2, {Sum[k, {1, 4}], 1, 4}]
```

```
Unprotect[Sum]; Sum[Sum[k, {1, 4}]^2, {Sum[k, {1, 4}], 1, 4}]
```

```
Solve[Positive[x]^2 == 1, Positive[x]]
```

```
Integrate[x[1], {x, 0, 2}, {x[1], -1, 1}]
```

```
Sum[x[1], {x, 0, 2}, {x[1], -1, 1}]
```

- c) What will be the result of the following input?

```
Unprotect[Message];
```

```
Message /: Message[___] := Null /; (Abort[]; False);
```

```
Integrate[1/(Sqrt[C^2] - C), {C, -1, 1}]
```

- d) Find a short (surely less than 20 characters) symbolic input that results in a mathematically wrong result. Do not use any variables or approximative numbers.

- e) Why does the following input (mathematically equal to 1) generate messages, instead of returning just 0?

```
t[x_] := ((x + 1)^2 - x^2 - x - 1)/x
t'[0]
```

f) What will be the result of the following input?

```
Block[{E}, D[E[x], x] /. head_[arg_] := arg[head]]
```

g) Find a rational function  $r(x, y, z)$  (with rational coefficients) such that `Together` does not act idempotent on it (meaning `Together[r(x, y, z)]` and `Together[Together[r(x, y, z)]]` are different).

h) Predict the result of the following input:

```
f1 = Factor[(x[2] - x[1])^3];
f2 = Factor[(x[2] - x[3])^3];
x[1] = x[3];
f1 - f2 === 0
```

i) Is there a *Mathematica* function (from the `System`` context) that, independently from any current and further progress in *Mathematica*, one will always be able to fool to give wrong result?

j) The function `Developer`ZeroQ` tries quickly to determine if an expression is identical to zero. Often it will correctly determine if an expression is zero, but it might sometimes give wrong results. (In physics terminology, one would call `Developer`ZeroQ` a FAPP-function [140★], [75★]; for PEF see [1339★].) For exact, numeric input this function will, among other techniques, use high-precision numericalization to find this out. Find a short (surely less than 10 characters) expression for which `Developer`ZeroQ` erroneously asserts that it is zero.

k) Find a function  $f(x, y)$ , such that *Mathematica* can evaluate `Integrate[f(x, y), {x, 0, 1}, {y, 0, 1}]` in closed form, but cannot evaluate `Integrate[f(x, y), {y, 0, 1}, {x, 0, 1}]` in closed form.

l) Predict the result of the following inputs:

```
makeDef1[d_, f_, A_] :=
  f /: d[1][f] /; (clearDef1[d, f, A]; makeDef2[d, f, A]; False) := Null
```

```
clearDef1[d_, f_, A_] :=
  f /: d[1][f] /; (clearDef1[d, f, A]; makeDef2[d, f, A]; False) =.
```

```
makeDef2[d_, f_, A_] := d /: HoldPattern[d[1][f][0]] :=
  (clearDef2[d, f]; makeDef1[d, f, A]; A)
```

```
clearDef2[d_, f_] := d /: HoldPattern[d[1][f][0]] =.
```

```
makeDef1[Derivative, f, f0];
D[f[x], x] /. x -> 0
```

m) Write a function that tries to find functions  $f(x)$  that are compositions of integer powers, exponential, and logarithmic functions, such that `Limit[f(x), x -> 0]` stays unevaluated.

n) Can you find a rational function in trigonometric functions for which the built-in `Integrate` cannot find the indefinite integral, but can after a substitution of variables?

o) Find an example of a quadratic polynomial  $p$  in the variable  $x$  with exact, numeric coefficients, such that `Solve[p == 0, x]` gives a mathematically wrong result.



p) What is wrong, from a scoping point of view, with the following naive definition of the Fourier transform  $\mathcal{F}_t[f(t)](\omega) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} \exp(i\omega t) f(t) dt$ ?

```
myFourierTransform[f_, t_, ω_, opts___] :=
  1/Sqrt[2 Pi] Integrate[f Exp[I t ω], {t, -Infinity, Infinity}, opts]
```

q) Find pairs of univariate functions  $f$  and their inverses  $f^{-1}$ , such that

- $f(f^{-1}(z)) = f^{-1}(f(z)) = z$  holds for all complex  $z$
- $f(f^{-1}(z)) = f^{-1}(f(z)) = z$  holds for almost all complex
- $f(f^{-1}(z)) = z$  holds for all complex  $z$ , but  $f^{-1}(f(z)) = z$  does not
- neither  $f(f^{-1}(z)) = z$  nor  $f^{-1}(f(z)) = z$  holds for all complex  $z$ .

r) Why does the following input give a mathematically wrong result?

```
Simplify[x DiracDelta[x], x == 0]
```

s) Motivate symbolically the result of the input

```
NIntegrate[Sin[x] x^(3/2), {x, 0, Infinity}, Method -> Oscillatory].
```

What is the exact value of this result?

### 33.<sup>L2</sup> 2D Newton–Leibniz Example, 1D Integral, Square Root of Differential Operator

a) Consider the following double integral:

$$\int_0^1 \int_0^1 \sqrt{(x-y)^2} dx dy.$$

Substituting limits in the (double) indefinite integral does not give the right result, despite the fact that the integrand and the (double) indefinite integral are continuous functions. How can one “fix” the double indefinite integral by doing the indefinite integrals?

b) Calculate the value of the integral  $\int_0^{\infty} \exp(-2x) (\coth(x) - 1/x) dx$  through its indefinite integral.

c) Compositions of the differential operator  $\partial/\partial x$  can be formally defined through the two symbolic identities [1929★], [714★], [1861★], [795★], [108★], [796★], [1336★], [683★], [814★], [1359★]

$$\frac{\partial^i}{\partial x^i} \left( \frac{\partial^j}{\partial x^j} \cdot \right) = \frac{\partial^{i+j}}{\partial x^{i+j}}.$$

$$\frac{\partial^i}{\partial x^i} (f(x) \cdot) = \sum_{k=0}^{\infty} \binom{i}{k} f^{(k)}(x) \frac{\partial^k}{\partial x^k}.$$

representing order independence and the Leibniz rule.

Here  $\partial^i/\partial x^i$  for negative  $i$  are understood as the inverse positive  $i$ , meaning  $\partial^i/\partial x^i (\partial^{-i} \cdot / \partial x^{-i}) = \text{identity}(\cdot)$ . (Practically this means that  $\partial^{-1}/\partial x^{-1}$  represents one-time indefinite integration  $[\partial^{-1} \cdot / \partial x^{-1} = \int_{-\infty}^x \cdot dx]$  [683★], [1567★], [360★] and the Leibniz rule represents partial integration in this formalism.)

Use these definitions to calculate the first ten  $\alpha_k$  of the square root [441★], [484★], [1589★], [1917★], [1804★]

$$\sqrt{\mathcal{L}} = \frac{\partial}{\partial x} + \sum_{k=0}^{\infty} \alpha_{-k}(x) \frac{\partial^{-k}}{\partial x^{-k}}.$$

where  $\mathcal{L}$  is the differential operator  $\mathcal{L} = \partial^2 + u(x)$ , containing an unspecified function  $u(x)$ .

### 34. L<sup>2</sup> Coefficients = Roots of a Univariate Polynomial, Amoebas, Tiling

a) Find all polynomials  $x^3 + ax^2 + bx + c$  that have  $a, b, c$  as their roots. Find the corresponding coefficients/roots for higher-order polynomials and visualize the coefficients/roots in the complex plane.

b) The amoeba of a system of polynomial equations  $p_j(z_1, z_2, \dots, z_n) = 0$ ,  $j = 1, \dots, m$  is the image of all solutions  $\{z_1, z_2, \dots, z_n\}$  under the map  $\{z_1, z_2, \dots, z_n\} \rightarrow \{\log(|z_1|), \log(|z_2|), \dots, \log(|z_n|)\}$  [1801★], [1726★], [1271★], [1270★], [1272★], [1516★], [713★]. Describe and visualize the amoeba of the equation  $w = 1 + 2z - z^3$ .

c) A bivariate function  $f(x, y)$  with  $\lim_{|x|+|y| \rightarrow \infty} f(x, y) = \infty$  induces a tiling of the plane with a tile defined as the set of all points  $\{x, y\}$ , such that  $|f(x, y)| \leq |f(x+i, y+j)|$  for all points  $\{i, j\}$ ,  $i, j \in \mathbb{Z}$  of a square lattice the plane [456★]. Find an exact parametric description for the tile in case  $f(x, y) = (3x+y)(y+3x)$  (this example comes from [456★]). Calculate the volume of the tile through integration and visualize the resulting tiling.

### 35. L<sup>2</sup> Cartesian Leaf Area, Triple Integral, Average Distance

a) Calculate the 2D area given by  $x^3 - 3yx + y^3 < 0$  in the first quadrant [514★].

b) Find the value of the following integral [809★]:

$$\int_0^1 \int_0^1 \int_0^1 \frac{1}{(1+x^2+y^2+z^2)^2} dx dy dz$$

Use a spherical coordinate system to calculate the integral.

c) Find the value of the following integral [558★]:

$$\int_0^{\infty} \int_0^{\infty} (x^2 + xy + y^2)^y e^{-(x+y)} dx dy$$

d) Determine analytically the average distance between two randomly selected points in the unit square [539★]. Use the independence of the components of the Cartesian coordinates to determine the probability that two randomly selected points in the interval  $(0, 1)$  are separated by a distance  $l$ . Find the average distance of two randomly chosen points in a 3D unit cube [1720★], [1228★].

e) The April 2003 issue of the *American Mathematical Monthly* contains the problem to calculate [559★]

$$I(a, b, c) = \int_0^{\infty} \int_0^{\infty} \int_0^{\infty} \frac{e^{-x-y-z} \sin(ax + by + cz)}{\sqrt{x+y+z}} dz dy dx.$$

Write a one-liner that calculates this integral. Simplify the result for real  $a, b, c$  and calculate the exact value of  $I(1, 1, 1)$ .

f) Calculate the following triple integral:

$$\int_0^{\infty} \int_0^x \int_0^y \frac{2 \cos(x) - \cos(x-y-z) - \cos(x-y+z)}{y^2 (x-z)^2} dz dy dx.$$

### 36.<sup>L2</sup> Duffing Equation, Secular Terms

a) Given the differential equation (Duffing equation) [959★], [56★], [1623★], [1021★], [974★], [53★]

$$\begin{aligned} y''(t) + y(t) + \epsilon y(t)^3 &= 0 \\ y(0) = 0, \quad y'(0) &= 0 \end{aligned}$$

( $\epsilon$  is a small parameter) using an ansatz of the form  $y(t) = \sum_{i=0}^n \epsilon^i y_i(t)$  calculate the first six terms  $y_i(t)$  [1625★]. Compare with the exact solution for  $\epsilon = 1/10$ .

Derive the first three orders for general initial conditions [1396★], [1202★].

b) Frequently, one is interested in periodic solutions of differential equation. Consider, for instance, the following nonlinear differential equation [1909★]

$$\Omega^2 \frac{\partial^2 X(t)}{\partial t^2} + \omega_0^2 X(t) = \sum_{k=2}^{\infty} J_k X(t)^k.$$

Here  $\Omega$ ,  $\omega_0$ , and the  $J_k$  are given parameter. Assume we can expand  $\Omega$  and  $X(t)$  naturally in a power series in  $\epsilon$ :

$$\begin{aligned} \Omega &= \sum_{k=0}^{\infty} \epsilon^k \omega_k \\ X(t) &= \epsilon \sum_{k=0}^{\infty} \epsilon^k x_k(t). \end{aligned}$$

For the lowest-order solution, we take  $x_0(t) = c_{0,c} \cos(t)$ . The differential equations for the  $x_k(t)$  are inhomogeneous harmonic oscillator differential equations with solutions  $x_k(t) = c_{k,c} \cos(t) + c_{k,s} \sin(t) + x_k^{(\text{inh})}(t)$ . Calculate conditions for the first 10 of the  $\omega_k$ , such that the  $x_k(t)$  become periodic functions.

### 37.<sup>L2</sup> Implicitization of Various Surfaces

Calculate polynomial implicit representations  $p(x, y, z) = 0$  for the following five surfaces:

- A “spindle” (come up with your own parametric description of a spindle).
- A cube-rooted sphere (this means a surface obtained by taking the third root (in case of negative values  $\xi$ , take  $-(-\xi)^{1/3}$  of the coordinate values of a sphere) [1923★].
- A cubed sphere (this means a surface obtained by taking the third power of the coordinate values of a sphere).
- A torus with a cross section of a cubed circle, in which the cubed circle is rotated when moved along the “outer” circle.
- A circle that is rotated around its diameter and its radius changes periodically.

Use `ContourPlot3D` to make pictures of all calculated implicit surfaces.

### 38.<sup>L2</sup> Riemann Surface of Kronig–Penney Dispersion Relation

Make a picture of the imaginary part of  $K = K(e)$ , where  $K(e)$  is defined implicitly by [1671★]

$$\cos(K) = \cos(\sqrt{e}) + \frac{4}{\sqrt{e}} \sin(\sqrt{e}).$$

Include all sheets of the Riemann surface in the picture, and let the region of the complex  $e$ -plane be  $-10 \leq \operatorname{Re}(e) \leq 60$ ,  $-10 \leq \operatorname{Im}(e) \leq 10$ .

(This equation comes up in the quantum-mechanical treatment of a particle in a periodic potential; and it is the eigenvalue equation of the Kronig–Penney model [1064★], [38★].)

### 39.<sup>L2</sup> Envelopes of Secants in an Ellipse, Lines Intersecting Four Lines

a) Given an ellipse  $x^2 + 4y^2 - 4 = 0$ , imagine all possible line segments with a start point and an end point on this ellipse, such that the length of the line segments is exactly 1. These line segments envelope a closed region inside the ellipse. Calculate the implicit representation of this region. Visualize how this region becomes formed by the enveloping line segments.

b) Given four generic lines in  $\mathbb{R}^3$ , how many lines (generically) exist that cross all four lines? (See [1459★], [867★], [1651★], and [1725★]; for similar problems see [1650★] and [1652★].)

### 40.<sup>L2</sup> Shortest Path in a Triangle Billiard

Given the triangle  $P_1P_2P_3$  with vertices  $P_1 = \{0, 0\}$ ,  $P_2 = \{1, 0\}$ ,  $P_3 = \{1, 2\}$ . Now, imagine a ball that starts at a point  $Q$  inside the triangle bounces against wall  $P_1P_2$ , is reflected there, bounces against wall  $P_2P_3$ , is reflected there, bounces against  $P_3P_1$  and comes back to the point  $Q$ . Calculate the exact value of the smallest length of such a path [514★].

### 41.<sup>L2</sup> Differential Equation Singularities, Weak Measurement Identity, Logarithmic Residue

a) Find a numerical approximation for the distance of the nearest singularity of

$$\begin{aligned} y'(x) &= 1 - xy(x)^2 \\ y(0) &= 0 \end{aligned}$$

from the origin [145★].

b) In [1772★], [24★], [25★], [1515★], [223★], [1646★], [1647★] (see also [534★]) the following peculiar identity was given ( $\eta$  is a real variable):

$$\sum_{k=0}^n c_k^{(n)}(\eta) f(x - d_k^{(n)}) \approx f(x - \eta)$$

Here the shifts  $d_k^{(n)}$  and the weights  $c_k^{(n)}(\eta)$  are given by

$$\begin{aligned} d_k^{(n)} &= \frac{k}{n} \\ c_k^{(n)}(\eta) &= \binom{n}{k} \eta^k (1 - \eta)^{n-k}. \end{aligned}$$

(The identity is peculiar because the superposition of shifted copies of  $f$  with, for  $|\eta| > 1$  large coefficients approximates another shifted copy of  $f$ .)

Assuming a Fourier expansion of  $f(x)$  exists, show that for  $n \rightarrow \infty$ , exact equality holds. Under which conditions does the identity hold approximately for finite  $n$ ?

c) Let  $f(z) = \sum_{k=-n}^{\infty} c_k z^k$  for some positive integer  $n$ . Then we have the residue  $\text{res}_{z=0}(f(z)) = c_1$ . For  $1 \leq n \leq 10$ , express the residue as a function of  $F(0)$  and  $\Phi^{(k)}(0)$  where  $F(z) = z^n f(z)$  and  $\Phi(z) = F'(z)/F(z)$  [1163★].

#### 42. L<sup>2</sup> Geometry Puzzle

Let ABC be a triangle. The sides  $\overline{AB}$  and  $\overline{AC}$  have the same length. A line starting from C intersects the line AB at the point D, and a line starting from B intersects the line AC at the point E. The following angles are given:  $\angle EBC = 60^\circ$ ,  $\angle BCD = 70^\circ$ , and  $\angle ABE = 20^\circ$ . Determine the angle  $\angle CDE$ . Here is a sketch of the problem:

Determine the angle  $\angle CDE$ . From [1127★], see also <http://www.dcs.st-andrews.ac.uk/~ad/mathrecs/advent/advent.html>.

#### 43. L<sup>2</sup> Differential Equation for Polynomial, Graph Eigenvalues

a) Given a polynomial  $p(x, y)$  in two variables, the  $y$  in  $p(x, y) = 0$  can be viewed as an implicitly defined function of  $x$ . Write a program, in which given an explicit bivariate polynomial  $p(x, y)$ , it derives a linear differential equation for  $y(x)$  [1053★], [1054★], [1056★], [383★], [384★].

b) Calculate the eigenvalues of the Laplace operator for the graph formed by the vertices (nodes) and edges (connections between nodes) of a stellated icosahedron. The action of Laplace  $\Delta$  operator on a function  $f$  at node  $q$  of a graph is given by [738★], [429★], [173★], [277★], [927★], [1488★], [216★]

$$\Delta f(q) = \text{numberOfNeighborsOf}q f(q) - \sum_{\text{neighbor nodes of } q} f(p).$$

c) Conjecture exact values for the smallest and the largest eigenvalues of the Laplace operator for the graph formed by the vertices (nodes) and edges (connections between nodes) of the 120-cell (see Exercise 17 of Chapter 2 of the Graphics volume [1751★]).

#### 44. L<sup>2</sup> Fourier Transform Eigenvalues, $\int_{-\infty}^{\infty} \theta(x) \delta(x) dx$ , $\delta^{(n)}(f(x))$ , PDF for Sums and Determinants, Fourier Transform and Series, Functional Differentiation

a) The eigenfunctions of the Fourier transform are of the form  $\exp(-x^2/2) \sum_{k=0}^n c_k x^k$ . Find the eigenvalues and eigenfunctions corresponding to  $0 \leq n \leq 12$ .

b) Find explicit sequences  $\delta_\varepsilon(x)$  and  $\theta_\varepsilon(x)$  such that  $\lim_{\varepsilon \rightarrow 0} \delta_\varepsilon(x) = \delta(x)$  and  $\lim_{\varepsilon \rightarrow 0} \theta_\varepsilon(x) = \theta(x)$  and  $\int_{-\infty}^{\infty} \delta_\varepsilon(x) \theta_\varepsilon(x) dx$  takes on different values depending on how fast  $\varepsilon$  and  $\epsilon$  approach 0. (This shows that  $\int_{-\infty}^{\infty} \delta(x) \theta(x) dx$  is not a well-defined integral.)

c) Let  $\xi$  be the only simple zero of  $f(x) = 0$ . Using the following three formulas [987★]:

$$g(x) \delta^{(n)}(x - \xi) = \sum_{k=0}^n (-1)^k \binom{n}{k} g^{(k)}(\xi) \delta^{(n-k)}(x - \xi),$$

$$\delta(f(x)) = \frac{\delta(x - \xi)}{|f'(\xi)|},$$

$$\delta^{(n)}(f(x)) = \frac{1}{f'(x)} \frac{\partial}{\partial x} \delta^{(n-1)}(f(x)),$$

find expansions for  $\delta^{(n)}(f(x))$  of the form  $\delta^{(n)}(f(x)) = \sum_{k=0}^n c_k(\xi) \delta^{(k)}(x - \xi)$  for  $2 \leq n \leq 10$ . Check some of the resulting formulas numerically.

**d)** The probability density  $p_z(\xi)$  for a sum  $z = x + y$  of two random variables  $x$  and  $y$  with distribution functions  $p_x(\xi)$  and  $p_y(\xi)$  is given by [215★], [521★], [1925★], [1227★], [1629★], [482★]

$$p_z(\xi) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} p_x(s) p_y(t) \delta(\xi - s - t) ds dt.$$

(This can also be viewed as a rewritten definition for B-splines.) Use this formula to calculate the distribution functions for  $n$  ( $n = 2, \dots, 5$ ) uniformly in  $[0, 1]$  distributed random numbers [1860★].

**e)** Calculate the probability distribution of the determinant of a  $2 \times 2$  matrix with random, uniform in  $[0, 1]$  distributed elements. Carry out a numerical simulation, and compare it with the theoretical distribution.

**f)** The divided differences  $[x_1 x_2 \dots x_n]$  of a function  $f$  at the points  $x_1, \dots, x_n$  have the integral representation [973★], [1275★], [457★]

$$[x_1 x_2 \dots x_n] = \int_0^{\infty} \int_0^{\infty} \dots \int_0^{\infty} \delta(1 - (x_1 + \dots + x_n)) f^{(n-1)}(\tau_1 x_1 + \tau_2 x_2 + \dots + \tau_n x_n) dx_n \dots dx_2 dx_1.$$

Use this formula to calculate  $[x_1 x_2 \dots x_8]$ .

**g)** Calculate the limits  $\lim_{\varepsilon \rightarrow 0} f_{\varepsilon}^{(\xi)}(x)$  and  $\lim_{\varepsilon \rightarrow 1} f_{\varepsilon}^{(\xi)}(x)$  where [469★], [1033★], [1304★]

$$f_{\varepsilon}^{(\xi)}(x) = \frac{1}{2\sqrt{\pi}\sqrt{1-\varepsilon}} e^{\frac{i\pi}{4}} e^{-\frac{i}{2} \frac{\varepsilon x^2 - 2\xi x + \xi^2}{1-\varepsilon}}.$$

Derive a first-order and an  $x$ -free differential equation for  $f_{\varepsilon}^{(\xi)}(x)$ .

**h)** Given the Fourier transform  $F^{(L)}(k) = (2\pi)^{-1/2} \int_{-L}^L \exp(ikx) f(x) dx$  of a function  $f(x)$ , visualize how the Fourier transform  $F_o^{(L)}(k)$  of  $2o + 1$  periodic continuations of  $f(x)$

$$F_o^{(L)}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp(ikx) f_o(x) dx$$

$$f_o(x) = \sum_{j=-o}^o \theta(x - (2jL - L)) \theta((2jL + L) - x) f(x + 2jL)$$

approaches the Fourier series coefficients  $c_n^{(L)} = 1/(2L) \int_{-L}^L \exp(inx\pi/L) f(x) dx$  for  $o \rightarrow \infty$  [1481★]. Use  $f(x) = \exp(-x^2)$  as the example function.

**i)** The functional derivative of a functional  $F[f(x)]$  is defined through (see for instance [775★], [175★], [1031★], [737★], [1653★], [906★], [1809★], [913★])

$$\frac{\delta F[f(x)]}{\delta f(y)} = \lim_{\epsilon \rightarrow 0} \frac{F[f(x) + \epsilon \delta(x - y)] - F[f(x)]}{\epsilon}.$$

Implement a function that attempts the functional differentiation for a given functional  $F[f(x)]$ . Use this function to calculate

$$\frac{\delta}{\delta f(y)} \int_{-\infty}^{\infty} f(x)^3 f'(x)^2 f''(x) dx .$$

Defining the Korteweg–de Vries bracket  $\{F, G\} = \int_{-\infty}^{\infty} \delta F(y) / \delta u(y) \partial(\delta F(y) / \delta u(y)) / \partial y dy$  [1219★], show that  $\{Q_i, Q_j\} = 0$  where

$$\begin{aligned} Q_0 &= \int_{-\infty}^{\infty} u(x) dx \\ Q_1 &= \int_{-\infty}^{\infty} \frac{1}{2} u(x)^2 dx \\ Q_2 &= \int_{-\infty}^{\infty} \left( \frac{1}{2} u'(x)^2 - u(x)^3 \right) dx \\ Q_3 &= \int_{-\infty}^{\infty} \left( \frac{5}{2} u(x)^4 - 5 u(x) u'(x)^2 + \frac{1}{2} u''(x)^2 \right) dx. \end{aligned}$$

Implement multiple functional differentiation defined through

$$\frac{\delta^n F[f(x)]}{\delta f(y_1) \cdots \delta f(y_n)} = \frac{\delta}{\delta f(y_1)} \left( \frac{\delta^{n-1} F[f(x)]}{\delta f(y_2) \cdots \delta f(y_n)} \right)$$

and calculate

$$\frac{\delta^3 \exp\left(\int_{-\infty}^{\infty} f(x) h(x) dx\right)}{\delta f(y_1) \delta f(y_2) \delta f(y_3)} \Big|_{f(y)=0} .$$

### 45. L2 Operator Splitting of Order 5

For many applications, it is useful to decompose exponentials of sums of operators into a product of exponentials of only one operator. (Examples are the solution of the time-dependent Schrödinger equation and the calculation of higher-order Runge–Kutta formulas for the solution of ordinary differential equations.) Calculate the real-valued coefficients  $\omega_1, \omega_2, \omega_3, \omega_4, \omega_5, \omega_6,$  and  $\omega_7$  of the fifth-order splitting formula [517★], [662★], [351★], [1242★], [1366★], [1894★], [1924★], [1569★], [1706★], [184★], [1315★], [1269★], [1005★], [1006★], [1268★], [352★], [1707★], [1471★], [1365★], [998★], [353★], [744★]:

$$e^{t(\hat{A}+\hat{B})} = e^{t\omega_1 \hat{A}} e^{t\omega_2 \hat{B}} e^{t\omega_3 \hat{A}} e^{t\omega_4 \hat{B}} e^{t\omega_5 \hat{A}} e^{t\omega_6 \hat{B}} e^{t\omega_7 \hat{A}} + O(t^5).$$

Here,  $\hat{A}$  and  $\hat{B}$  are the two (in general noncommuting) operators.

### 46. L2 Maximal Triangle Area and Tetrahedron of Maximal Volume

a) Given three concentric circles of radius  $r_1, r_2,$  and  $r_3,$  calculate the maximal area of the triangle that has one vertex at each of the circles. For  $r_1 = 1, r_2 = 2, r_3 = 3,$  calculate the explicit value of the area [645★].

b) Given the areas of the four faces of a tetrahedron, find the maximal volume that the tetrahedron can have. Express the result in a compact way. For the two sets of four areas,  $\{\frac{9}{10}, \frac{10}{10}, \frac{11}{10}, \frac{12}{10}\}$  and  $\{1, 1, 1, 1\},$  calculate a closed-form symbolic result for the maximal volume. [717★], [42★], [850★]

# CHAPTER 2

## Exercises

### 1.<sup>L1</sup> Generating Function for $T_n(x)$ , Mehler's Formula, Bauer–Rayleigh Expansion, and More

a) Verify the first few terms in the following series expansion:

$$e^{zx} \cosh(z\sqrt{x^2-1}) = \sum_{n=0}^{\infty} \frac{T_n(x)}{n!} z^n.$$

Using the trigonometric representations of the Chebyshev polynomials, also prove this relation symbolically.

b) Check Mehler's formula for the lowest-order terms:

$$\frac{1}{\sqrt{1-a^2}} \exp\left(-\frac{(z^2+z'^2-2zz'a)}{1-a^2}\right) = \exp(-(z^2+z'^2)) \sum_{n=0}^{\infty} \frac{a^n}{2^n n!} H_n(z) H_n(z').$$

c) Check the first few terms (in  $x$ ) for the Bauer–Rayleigh expansion:

$$e^{ixy} = \sqrt{\frac{\pi}{2x}} \sum_{l=0}^{\infty} i^l (2l+1) J_{l+1/2}(x) P_l(y).$$

Here,  $J_\nu(z)$  is the Bessel function of order  $\nu$ . (For a short derivation, see [564★] and [216★]; for generalizations, see [500★], for pitfalls, see [382★].)

d) Verify the first few terms of the following addition theorem for the Hermite polynomials:

$$\sum_{m=0}^n \frac{n!}{m!(n-m)!} H_{n-m}(\sqrt{2}z) H_m(\sqrt{2}z') = 2^{n/2} H_n(z+z').$$

e) Verify the correctness of the following relations for the Chebyshev polynomials of the first kind for the first few  $n$ :

$$\begin{aligned} 2T_m(x)T_n(x) &= T_{m+n}(x) + T_{m-n}(x) \quad (m > n) \\ 2T_n(x)^2 &= 1 + T_{2n}(x). \end{aligned}$$

Using the trigonometric representations of the Chebyshev polynomials, prove this relation symbolically as well.

f) Verify the following formula for the products of Legendre polynomials [327★], [462★], [397★] for some  $n$  and  $m$ :

$$P_m(x)P_n(x) = \sum_{l=|m-n|}^{m+n} b_{lmn} P_l(x).$$

The coefficients  $b_{lmn}$  are given by the following expression:



$$b_{lmn} = \begin{cases} (2l+1) \frac{(m+n-l-1)!! (l+n-m-1)!! (m+n+l)!! (l+m-n-1)!!}{(m+n-l)!! (l+n-m)!! (m+n+l+1)!! (l+m-n)!!} & l+m+n \text{ even} \\ 0 & \text{otherwise.} \end{cases}$$

g) Check the following formula for Laguerre polynomials [475★] for some  $n$ :

$$L_n(z) = (-1)^n \frac{e^z}{n!} \left( z \frac{d^2}{dz^2} + \frac{d}{dz} \right)^n e^{-z}.$$

h) The zeros  $x_k^{(n)}$  of the Hermite polynomials  $H_n(x)$  fulfill the following nice relation [6★], [119★], [120★]:

$$\sum_{k=1}^n \frac{1}{x_l^{(n)} - x_k^{(n)}} = x_l^{(n)}.$$

Check this relation for some  $n$ .

i) Define the following continued fraction  $R_k(\epsilon, x)$  with  $k$  occurrences of  $x$ .

$$R_k(\epsilon, x) = \frac{1}{1 - \frac{x}{1 - \frac{x}{1 - \frac{x}{1 - \epsilon x}}}}$$

Prove that  $R_k(\epsilon, x)$  has the following closed-form representation [385★]:

$$R_k(\epsilon, x) = \frac{1}{\sqrt{x}} \frac{U_{k-1}\left(\frac{1}{2\sqrt{x}}\right) - \epsilon \sqrt{x} U_{k-2}\left(\frac{1}{2\sqrt{x}}\right)}{U_k\left(\frac{1}{2\sqrt{x}}\right) - \epsilon \sqrt{x} U_{k-1}\left(\frac{1}{2\sqrt{x}}\right)}.$$

j) The 3D spherical harmonics  $Y_l^m(\vartheta, \varphi) = ((2l+1)/(4\pi)(l-m)!/(l+m)!)^{1/2} P_l^m(\cos(\vartheta)) e^{im\varphi}$  (in *Mathematica* `SphericalHarmonicY[l, m, \vartheta, \varphi]`) can, for nonnegative integers  $l$  and  $m$ , be written in the form  $Y_l^m(\vartheta, \varphi) = c_{l,m}(x^2 + y^2 + z^2)^{-l} p(x, y, z)$  where  $c_{l,m}$  is a numerical constant and  $p(x, y, z)$  is a homogeneous polynomial of degree  $l$  over the Gaussian integers [589★], [616★], [302★], [423★], [17★]. Write a one-liner that writes a given `SphericalHarmonicY[l, m, \vartheta, \varphi]` in this form.

k) Implement a one-liner that implements the calculation of the first  $n$  spherical harmonics

$$\mathcal{Y}_l(\vartheta, \varphi) = \{\{Y_{0,0}(\vartheta, \varphi)\}, \{Y_{1,-1}(\vartheta, \varphi), Y_{1,0}(\vartheta, \varphi), Y_{1,1}(\vartheta, \varphi)\}, \dots, \{Y_{l,-l}(\vartheta, \varphi), \dots, Y_{l,l}(\vartheta, \varphi)\}\}$$

that is based on the recursion [181★], [539★], [589★]

$$\begin{aligned} \mathcal{Y}_{l,m}(\vartheta, \varphi) &= \frac{1}{l-m} (\cos(\vartheta) \mathcal{Y}_{l-1,m} + (\cos(\varphi) \sin(\vartheta) - i \sin(\varphi) \sin(\vartheta)) \mathcal{Y}_{l-1,m+1}) \text{ for } m \leq 0 \\ \mathcal{Y}_{l,m}(\vartheta, \varphi) &= (-1)^m \overline{\mathcal{Y}_{l,-m}(\vartheta, \varphi)} \\ \mathcal{Y}_{1,-1}(\vartheta, \varphi) &= (\cos(\varphi) \sin(\vartheta) - i \sin(\varphi) \sin(\vartheta)) / 2 \\ \mathcal{Y}_{1,-1}(\vartheta, \varphi) &= \cos(\vartheta) \\ \mathcal{Y}_{1,1}(\vartheta, \varphi) &= -(\cos(\varphi) \sin(\vartheta) + i \sin(\varphi) \sin(\vartheta)) / 2. \end{aligned}$$

The normalized spherical harmonics are then given by

$$Y_{l,m}(\vartheta, \varphi) = \sqrt{\frac{(2l+1)(l+m)!(l-m)!}{4\pi}} \mathcal{Y}_{l,m}(\vartheta, \varphi).$$

For machine-precision  $\vartheta$  and  $\varphi$ , implement a compiled version. To which precision can you calculate  $Y_l(\vartheta, \varphi)$  using the compiled version?

## 2.<sup>L2</sup> Generalized Fourier Series

Examine the convergence of the generalized Fourier series in terms of the classical orthogonal polynomials for the function  $f(z) = \theta(z)(1 - \theta(z))$ .

## 3.<sup>L1</sup> Transmission Through Layers, Sums of Zeros

a) Graphically examine the function

$$t(k) = \frac{1}{1 + k^2 U_n(\cos(k) + \sin(k)/k)^2} \quad n = 0, 1, 2, \dots, k \geq 0$$

where  $U_n(z)$  are the Chebyshev polynomials.

b) Find a closed form for  $\sigma_o^{(n)} = \sum_{k=1}^n (z_k^{(n)})^o$  for positive integer  $n$  and  $o$  with  $n > o/2$  where  $z_k^{(n)}$  is the  $k$ th root of  $T_n(z)$ .

## 4.<sup>L1</sup> General Orthogonal Polynomials

Implement the following algorithm for the computation of the orthogonal polynomials corresponding to a weight function  $w(z)$  on the interval  $(a, b)$ . Let

$$c_{ij} = \int_a^b w(z) z^{i+j} dz$$

$$\Delta_n = \det \mathbf{C} \quad i, j = 0, 1, \dots, n$$

$$d_{ij}^{(n)} = \begin{cases} c_{ij}, & j < n \\ z^j, & j = n \end{cases}$$

$$\Gamma_n = \det \mathbf{D}^n \quad i, j = 0, 1, \dots, n.$$

Here,  $c_{ij}$  and  $d_{ij}^{(n)}$  are the elements of the matrices  $\mathbf{C}$  and  $\mathbf{D}$ .

Then, the nonnormalized form of the  $n$ th orthogonal polynomial  $p_n(z)$  corresponding to the weight  $w(z)$  is given by

$$p_n(z) = \frac{\Gamma_n}{\sqrt{\Delta_n \Delta_{n-1}}}$$

(See, e.g., [309★], [9★], [555★], [156★], [338★], and [217★]). Implement a normalization of the polynomials so that

$$\int_a^b p_n(z) p_m(z) w(z) dz = \delta_{nm}.$$

(One could also use the last equation for a direct recursive calculation of the  $n$ th orthogonal polynomial. Setting

$$p_n(z) = \sum_{i=0}^n a_i z^i$$

the orthogonality relations lead to a system of equations that can be solved for the  $a_i$  using `Solve`. However, since this system of equations is nonlinear (note the last equation), such an implementation would require a lot of unnecessary work. Another possibility would be to use Gram-Schmidt orthogonalization. A corresponding package is `LinearAlgebra`Orthogonalization``.)

## 5.1<sup>1</sup> Symmetric Polynomials

Symmetric polynomials, i.e., polynomials  $f(x_1, x_2, \dots, x_n)$  in several variables  $x_1, x_2, \dots, x_n$  for which  $f(x_1, x_2, \dots, x_n) = f(\pi(x_1, x_2, \dots, x_n))$ , where  $\pi(x_1, x_2, \dots, x_n)$  is an arbitrary permutation of the elements  $x_1, x_2, \dots, x_n$  holds, play a major role in algebra (see, e.g., [461★], [330★], [585★], [565★], [378★], [141★], [129★], [542★], [101★]; for physics applications, see [40★], [512★]). The most important symmetric polynomials are the following:

- the power sums  $S_k$

$$S_k(x_1, \dots, x_n) = \sum_{i=1}^n x_i^k, \quad k = 0, 1, \dots$$

- the discriminant  $D$

$$D(x_1, \dots, x_n) = \prod_{\substack{i,j=1 \\ i>j}}^n (x_i - x_j)^2$$

- the elementary symmetric polynomials

$$C_k(x_1, \dots, x_n) = \sum_{\substack{i_1, i_2, \dots, i_k=1 \\ i_1 < i_2 < \dots < i_k \leq n}} x_{i_1} x_{i_2} \cdots x_{i_k}, \quad k = 1, 2, \dots$$

- the Wronski polynomials

$$P_k(x_1, \dots, x_n) = \sum_{\substack{i_1, i_2, \dots, i_n=0 \\ i_1 + i_2 + \dots + i_n = k}} x_1^{i_1} x_2^{i_2} \cdots x_n^{i_n}, \quad k = 1, 2, \dots$$

- a) For a given list of variables `varList`, length  $n$ , and given order  $k$ , implement the computation of these polynomials. Try not to use temporary variables (including iterator variables in `Table`, etc.). Do not use

```
ElementarySymmetricPolynomials[k_Integer?(# >= 1&), varList_] :=
  Coefficient[Times @@ (C - #& /@ varList), C, k + 1]
```

or similar implementations.

- b) The following so-called Newton relations ([110★], [237★]) hold for the power sums and the elementary symmetric polynomials:

$$S_k(x_1, \dots, x_n) + \sum_{j=1}^{k-1} (-1)^j C_j(x_1, \dots, x_n) S_{k-j}(x_1, \dots, x_n) + (-1)^k k C_k(x_1, \dots, x_n) = 0, \quad k \leq n$$

$$S_k(x_1, \dots, x_n) + \sum_{j=1}^n (-1)^j C_j(x_1, \dots, x_n) S_{k-j}(x_1, \dots, x_n) = 0, \quad k > n.$$

Verify these relationships for  $n = 3$  and  $k < 5$ .

c) Show for some cases that the so-called Waring formula holds:

$$S_k(x_1, \dots, x_n) = \sum_{\substack{i_1, i_2, \dots, i_n=0 \\ i_1 + 2i_2 + 3i_3 + \dots + ni_n = k}} \frac{(-1)^{i_1 + i_2 + \dots + i_n} (i_1 + i_2 + \dots + i_n - 1)!}{i_1! i_2! \dots i_n!} C_1^{i_1} C_2^{i_2} \dots C_n^{i_n}.$$

d) Let  $S_k^{(j)}(x_1, \dots, x_n) = S_k^{(j)}(x_1, \dots, x_{j-1}, x_{j+1}, \dots, x_n)$  (meaning that the  $j$ th variable is removed from the  $n$  variables  $x_k$ ). Then the following identity holds [125★].

$$\sum_{j=1}^n S_k^{(j)}(x_1, \dots, x_n) = (\alpha n + \beta k + \gamma) S_k(x_1, \dots, x_n).$$

Determine the integers  $\alpha$ ,  $\beta$ , and  $\gamma$ .

e) The normalized elementary symmetric polynomials  $\tilde{C}_k(x_1, \dots, x_n) = n!(n-k)!C_k(x_1, \dots, x_n)/n!$  fulfill for real  $x_k$  the inequalities [441★], [396★], [438★]

$$\tilde{C}_{k-1}(x_1, \dots, x_n) \tilde{C}_{k+1}(x_1, \dots, x_n) \leq \tilde{C}_k(x_1, \dots, x_n)^2, \quad k = 1, \dots, n-1.$$

Verify these inequalities for  $2 \leq n \leq 4$ .

f) Using Vieta's relations from the above formulas, one can derive the following identity for the sum  $s_j$  of the  $j$ th powers

$$s_j = \sum_{i=1}^n x_i^j$$

of all roots  $x_i$  ( $i = 1, \dots, n$ ) of a polynomial equation  $a_0 x^n + a_1 x^{n-1} + a_2 x^{n-2} + \dots + a_{n-1} x + a_n = 0$ :

$$s_j = -j \frac{a_j}{a_0} - \sum_{k=1}^{j-1} s_k \frac{a_{k-j}}{a_0}.$$

For the  $s_j$ , a recursive implementation is obvious. In a functional style, implement a program that computes the first  $m$  of the  $s_j$  simultaneously. Try to avoid the use of any named variable. Use a polynomial and compare the result with a direct numerical calculation of the  $s_j$ .

## 6.<sup>L2</sup> Generalized Lissajous Figures, Hyperspherical Harmonics, Hydrogen Orbitals

a) Construct “generalized Lissajous figures” by replacing the classical  $\{\sin Or Cos(nt), \sin Or Cos(mt)\}$  by  $\{p_n(t), p_m(t)\}$ ,  $p_m(t)$  being an orthogonal polynomial. (The motivation for this choice of functions is the fact that  $\sin(nt)$  is an orthogonal function system, and the Sturm oscillation theorem holds (see, e.g., [463★]), which accounts for the “oscillation up and down and from right to left” of the resulting curves.)

b) Check the formula  $(\hat{\Lambda}^2 - \lambda(\lambda + d - 2)) C_\lambda^{(d-2)/2}(\mathbf{e} \cdot \mathbf{e}') = 0$  from the beginning of Section 2.4 for small  $d$  and  $\lambda$ .

For some small integers  $\lambda$ , show that the function

$$H_\lambda(\mathbf{r}, \mathbf{r}') = |\mathbf{r}|^\lambda \frac{C_\lambda^{(d-2)/2}\left(\frac{\mathbf{r} \cdot \mathbf{r}'}{|\mathbf{r}| |\mathbf{r}'|}\right)}{C_\lambda^{(d-2)/2}(1)}$$

fulfills the Laplace equation and that  $H_\lambda(\mathbf{e}', \mathbf{e}') = 1$  [48★].

Multidimensional spherical harmonics  $Y_{m_0}^{m_1, \dots, m_{d-2}}$  are defined as [48★], [631★], [364★], [440★], [193★], [172★], [83★], [164★]

$$Y_{m_0}^{m_1, \dots, m_{d-2}}(\vartheta_1, \vartheta_2, \dots, \vartheta_{d-2}, \phi) = e^{i m_{d-2} \phi} \prod_{k=0}^{d-3} \sin^{m_{k+1}}(\vartheta_{k+1}) C_{m_k - m_{k+1}}^{(d-k-2+2m_{k+1})/2}(\cos(\vartheta_{k+1})).$$

Here the  $0 \leq \vartheta_k \leq \pi$  are the polar angles in a  $dD$  spherical coordinate system  $\{r, \vartheta_1, \dots, \vartheta_{d-2}, \phi\}$ . The  $m_j$  are nonnegative integers fulfilling  $m_0 \geq m_1 \geq \dots \geq m_{d-2} \geq 0$ .

The angular part  $\Delta_\circ (= \hat{\Lambda}^2)$  of the  $dD$  Laplace operator  $\Delta$  in hyperspherical coordinates acts on a function  $f(\vartheta_1, \dots, \vartheta_{d-2}, \phi)$  in the following way [292★], [487★], [154★], [193★], [440★]:

$$\Delta_\circ f = \left( \sum_{k=0}^{d-3} \frac{\sin^{k-d+2}(\vartheta_{k+1})}{\prod_{j=1}^k \sin^2(\vartheta_j)} \frac{\partial}{\partial \vartheta_{k+1}} \left( \sin^{d-2-k}(\vartheta_{k+1}) \frac{\partial f}{\partial \vartheta_{k+1}} \right) \right) + \frac{1}{\prod_{j=1}^{d-2} \sin^2(\vartheta_j)} \frac{\partial^2 f}{\partial \phi^2}.$$

For small  $d, m_j$ , show that  $Y_{m_0}^{m_1, \dots, m_{d-2}}(\vartheta_1, \vartheta_2, \dots, \vartheta_{d-2}, \phi)$  are eigenfunctions of the angular part of the  $dD$  Laplace operator

$$-\Delta_\circ Y_{m_0}^{m_1, \dots, m_{d-2}}(\vartheta_1, \vartheta_2, \dots, \vartheta_{d-2}, \phi) = m_0(m_0 + d - 2) Y_{m_0}^{m_1, \dots, m_{d-2}}(\vartheta_1, \vartheta_2, \dots, \vartheta_{d-2}, \phi).$$

(For the 1D case, see [109★]; for  $\exp(i \tau \Delta_\circ)$ , see [371★].)

c) The (not normalized) probability density for finding an electron in a hydrogen atom that the state  $|n l m\rangle$  in spherical coordinates is  $p_{n,l}(r, \vartheta) = |e^{-r} r^l L_{n-l-1}^{2l+1}(2r) P_n^l(\cos(\vartheta))|^2$  [622★], [477★]. Show  $p_{12,6}(r, \vartheta) = c$  for various  $c$ .

### 7. L<sup>2</sup> Zeros of Hermite Polynomials, $q$ -Hermite Polynomials, Pseudodifferential Operator, Moments of Hermite Polynomial Zeros

a) The  $n$ th Hermite polynomial  $H_n(z)$  has  $n$  real zeros. Construct a visualization that shows what happens with the zeros of  $H_n(z)$  if  $n$  changes continuously from one integer value to the next. (The command `ND` from the package `NumericalMath`NLimit`` is very useful here.)

b) The  $q$ -Hermite polynomials  $H_n^{(q)}(z)$  [23★], [25★], [190★], [88★], [8★], [74★], [26★], [530★], [75★], [191★] can be defined in the following manner [281★], [372★]:

$$H_n^{(q)}(z) = 2z q^{-2n+3/2} H_{n-1}^{(q)}(z) - \frac{2}{q^2} \frac{(1 - \frac{1}{q^{2n-2}})}{(1 - \frac{1}{q^2})} H_{n-2}^{(q)}(z)$$

$$H_0^{(q)}(z) = 1$$

$$H_1^{(q)}(z) = 2q^{-1/2} z.$$

For small  $n$  calculate the positions and the order of the branch points of the function  $z(q)$  implicitly defined by  $H_n^{(q)}(z) = 0$  [640★]. Make an animation that visualizes the dependence of the zeros  $z_0(q)$  of  $H_n^{(q)}(z_0(q))$ . Vary  $r_q$  in  $q = r_q \exp(i \varphi_q)$  from frame to frame.

c) By using expansion in orthogonal polynomials, calculate the lowest eigenvalue of the following pseudodifferential equation to at least correct digits for  $m = 1$ . (This describes ground-state energy of a relativistic harmonic oscillator with mass  $m$  in a half space [582★], [214★], [498★], [253★], [204★], [254★], [255★], [431★], [344★], [490★], [222★], [223★], [376★], [147★], [100★]. But such-type Hamiltonians are not relativistically invariant [535★], [544★].))

$$\sqrt{m^2 + \frac{\partial^2}{\partial x^2}} \psi_\varepsilon(x) + x^2 \psi_\varepsilon(x) = \varepsilon \psi_\varepsilon(x)$$

$$\psi_\varepsilon(0) = 0.$$

Sketch the dependence of the eigenvalue as a function of  $m$ .

c) The moments  $\mu_m(n)$  of the  $n$  zeros  $z_k^{(n)}$ ,  $k = 1, \dots, n$  of the Hermite polynomials  $H_n(z)$  defined by

$$\mu_m(n) = \frac{1}{n} \sum_{k=1}^n (z_k^{(n)})^m$$

can be expressed as  $\mu_m(n) = \sum_{j=0}^{m/2} c_j^{(m)} n^j$  with rational  $c_j^{(m)}$  [13★]. Calculate the first few  $\mu_m(n)$ . Is it feasible to calculate  $\mu_{100}(n)$ ?

### 8.L1 Iterated Polynomial Substitution

Starting with the polynomial  $p(z) = \sum_{i=0}^n z^i$ , repeatedly replace the powers  $z^j$  by initially randomly chosen and then fixed polynomials (for instance, orthogonal polynomials) of order  $j$ . Calculate the zeros of the resulting polynomials and display them graphically.

### 9.L2 Hermite Polynomials, Coherent States, Isospectral Potentials, Wave Packets

Let  $\phi_n(x)$  be the normalized harmonic oscillator eigenfunctions

$$\phi_n(x) = \frac{1}{\sqrt{\sqrt{\pi} 2^n n!}} e^{-x^2/2} H_n(x).$$

a) Find the parameter  $\alpha$  such that the integral  $\int_{-\infty}^{\infty} \Psi(\alpha; x) \phi_k(x) dx$  becomes maximal (let  $k = 0, 2$ ). Here,  $\Psi(\alpha; x) \sim \exp(-\alpha x^4)$  and  $\int_{-\infty}^{\infty} \Psi(\alpha; x)^2 dx = 1$ .

b) Find the parameters  $\beta_j$ ,  $\gamma_j$ , and  $\xi_j$  such that the integral  $\int_{-\infty}^{\infty} \Psi(x) \phi_k(x) dx$  ( $k = 1, 3$ ) becomes maximal. Here,

$$\Psi(x) \sim \sum_{j=1}^2 \beta_j e^{-\gamma_j(x-\xi_j)^2} \text{ and } \int_{-\infty}^{\infty} \Psi(x)^2 dx = 1.$$

c) The harmonic oscillator eigenfunctions  $\phi_n(x)$  can be thought of as Fourier coefficients of time-dependent coherent states  $\psi_C(\alpha; x, t)$  [275★], [274★], [276★], [470★], [170★], [509★].

$$\phi_n(x) = \frac{1}{2\pi} \exp(|\alpha|^2) \frac{\sqrt{n!}}{\alpha^n} \int_0^{2\pi} \psi_C(\alpha; x, t) e^{(2n+1)/2it} dt.$$

The time-dependent coherent states for a harmonic oscillator are given by [510★], [326★], [503★], [294★]:

$$\psi_C(\alpha; x, t) = -\frac{(-1)^{3/4}}{\sqrt[4]{\pi}} \frac{\exp((-x^2 - \alpha^2 e^{-2it} + \bar{\alpha}^2 - 2\operatorname{Re}(\alpha)^2 + 2\sqrt{2} x \alpha e^{-it})/2)}{\sqrt{1 - i \cot(t)} \sqrt{\sin(t)}}.$$

For a given  $n$  and appropriately chosen  $\alpha$ , visualize how the harmonic oscillator eigenfunctions evolve from  $\int_0^T \psi_C(\alpha; x, t) e^{(2n+1)/2it} dt$  as a function of  $T$ . (For the evolution of the harmonic oscillator eigenfunction from extended wave functions, see [417★].)

d)  $P_{\text{qu}}(x) = |\phi_n(x)|^2$  describes the probability density of finding a harmonic oscillator quantum particle with energy  $2n + 1$  at position  $x$ . In the classical limit [485★], [73★], this probability tends to

$$P_{\text{cl}}(x) = \frac{\theta(x + \sqrt{2n + 1}) \theta(\sqrt{2n + 1} - x)}{\pi \sqrt{2n + 1 - x^2}}$$

[351★], [484★]. For a moderate large  $n$ , how good can an averaged  $P_{\text{qu}}(x)$ ,

$$\tilde{P}_{\text{qu}}(x; \varepsilon) = \frac{1}{2\varepsilon} \int_{x-\varepsilon}^{x+\varepsilon} P_{\text{qu}}(\xi) d\xi$$

[166★], [483★], [207★], [210★], [363★], and [571★] approximate  $P_{\text{cl}}(x)$ ? What is the optimal  $\varepsilon$ ?

e) The functions [211★]

$$\Psi_n(\alpha, z) = \frac{1}{\sqrt{n! L_n(1 - \frac{1}{\eta})}} \sum_{k=0}^n \left(\frac{1}{\eta} - 1\right)^{\frac{n-k}{2}} \frac{n!}{(n-k)! \sqrt{k!}} \phi_k(z)$$

interpolate smoothly between the harmonic oscillator eigenstates  $\phi_k(z)$  and the time-independent coherent states

$$\Phi(z; \alpha) = e^{-\alpha^2/2} \sum_{k=0}^{\infty} \frac{\alpha^k}{\sqrt{k!}} \phi_k(z).$$

In the limit  $\eta \rightarrow 1$ , we have  $\Psi_n(\alpha, z) = \phi_k(z)$ , and in the limit  $\eta \rightarrow 0$ ,  $n \rightarrow \infty$ ,  $n\eta^{1/2} = \alpha$ , we have  $\Psi_n(\alpha, z) = \Phi(z; \alpha)$ . Visualize this transition between  $\phi_{12}(z)$  and  $\Phi(z; 2)$ .

f) Given the eigenvalues  $\varepsilon_n$  and eigenfunctions  $\phi_n(z)$  of the eigenvalue problem

$$-\phi_n''(z) + V(z) \phi_n(z) = \varepsilon_n \phi_n(z),$$

an isospectral (meaning having the same eigenvalues) eigenvalue problem (the notation  $\psi_n[\phi_n](z; \lambda)$  indicates that  $\psi_n$  is a functional of  $\phi_n$ )

$$-\psi_n[\phi_n]''(z; \lambda) + \mathcal{V}[\phi_n](z; \lambda) \psi_n[\phi_n](z; \lambda) = \varepsilon_n \psi_n[\phi_n](z; \lambda)$$

can be constructed by the following Darboux transformation [92★], [491★], [404★], [374★], [329★], [403★], [492★], [319★], [479★], [452★], [489★], [415★], [320★], [34★], [414★], [493★], [325★]:

$$\psi_n[\phi_n](z; \lambda) = \sqrt{\lambda(\lambda + 1)} \frac{\phi_n(z)}{\int_{-\infty}^z \phi_n(z)^2 dz + \lambda}$$

$$\mathcal{V}[\phi_n](z; \lambda) = V(z) - \frac{d}{dz^2} \ln\left(\int_{-\infty}^z \phi_n(z)^2 dz + \lambda\right)^2.$$

The new (normalized) eigenfunctions  $\psi_n[\phi_n](z; \lambda)$  are functionals of the  $\phi_n(z)$  and  $\lambda$  is a free parameter.

Use for the  $\phi_n(x)$  the normalized harmonic oscillator eigenfunctions  $\phi_n(x)$ . Visualize some of the resulting  $\psi_n[\phi_n](z; \lambda)$  and  $\mathcal{V}[\phi_n](z; \lambda)$ . Make conjectures for the exact symbolic values of the following two integrals:

$$\int_{-\infty}^{\infty} (\psi_n[\phi_n](z; \lambda) - \phi_n(z))^2 dz$$

$$\int_{-\infty}^{\infty} (\mathcal{V}[\phi_n](z; \lambda) - V(z)) dz.$$

g) “Wave packets” can be formed by superimposing energy eigenstates. For the harmonic oscillator, one possible superposition is [361★], [362★]

$$\Psi_n^{(m)}(z) = \sum_{k=-m}^m \phi_{n-k}(z).$$

For  $n = 100$ , which  $m$  gives the most localized wave packet? Visualize the  $t$ -dependence of the state

$$\Psi_n^{(m)}(z, t) = \sum_{k=-m}^m \phi_{n-k}(z) e^{-i(2k+1)t}.$$

h) A possible generalization of the harmonic oscillator eigenfunctions to  $d$  dimensions is given by the following functions ( $d = 1$  yields the classical harmonic oscillator eigenfunctions  $\phi_n(x)$ ) [392★]:

$$\phi_n^{(d)}(x) = \frac{[n]_d!}{n!} \frac{1}{\sqrt{\sqrt{\pi} 2^n [n]_d!}} e^{-\frac{x^2}{2}} H_n^{(d)}(x).$$

Here  $H_n^{(d)}(x)$  are  $d$ -dimensional generalizations of the Hermite polynomials

$$H_n^{(d)}(x) = \frac{n!}{[n]_d!} (-1)^n e^{\frac{x^2}{2}} \left( \frac{\partial_d}{\partial_d x} \right)^n e^{-\frac{x^2}{2}}$$

and the  $d$ -dimensional derivative  $\partial_d \cdot / \partial_d x$  and factorial  $[n]_d!$  are defined by

$$\frac{\partial_d f(x)}{\partial_d x} = f'(x) + \frac{(d-1)}{2x} (f(x) - f(-x))$$

$$[n]_d! = \prod_{k=1}^n [n]_d = \prod_{k=1}^n \left( n + \frac{(d-1)}{2} (1 - (-1)^k) \right).$$

Calculate and visualize the first few  $\phi_n^{(d)}(x)$  as a function of  $d$ . (For the multidimensional harmonic oscillator in integer dimensions, see for instance [558★], [287★], [116★], [352★], [607★], [367★], [541★], [451★].)

### 10.<sup>L3</sup> High-Order Perturbation Theory, Eigenvalue Differential Equation

a) The Rayleigh–Schrödinger perturbation theory treats the following problem: Given a (linear) eigenvalue problem

$$(\hat{L}_0 + g \hat{V}) \psi_n^{(g)}(z) = \varepsilon_n^{(g)} \psi_n^{(g)}(z)$$

the perturbed eigenvalues  $\varepsilon_n^{(g)}$  and eigenfunctions  $\psi_n^{(g)}(x)$  are to be found. The unperturbed problem is

$$\hat{L}_0 \psi_n^{(0)}(z) = \varepsilon_n^{(0)} \psi_n^{(0)}(z)$$

and is assumed to be exactly solvable.  $g \hat{V}$  is the perturbation. One starts with expanding the eigenvalues  $\varepsilon_n^{(g)}$  and eigenfunctions  $\psi_n^{(g)}(z)$  in powers of  $g$  using the expansion coefficients  ${}^{(n)}\varepsilon_j$  and  ${}^{(n)}c_{j,k}$ .



$$\mathcal{E}_n^{(g)} = \sum_{j=0}^{\infty} g^j {}^{(n)}\mathcal{E}_j$$

$$\psi_n^{(g)}(x) = \sum_{j=0}^{\infty} g^j \left( \sum_{k=0}^{\infty} {}^{(n)}c_{j,k} \psi_k^{(0)}(z) \right).$$

Using the initial conditions  ${}^{(n)}\mathcal{E}_0 = \mathcal{E}_n^{(0)}$ ,  ${}^{(n)}c_{0,k} = \delta_{k,n}$ , and  ${}^{(k)}c_{j,k} = \delta_{j,k}$ , it is straightforward to derive the following recursion relations for the  ${}^{(n)}\mathcal{E}_j$  and  ${}^{(n)}c_{j,k}$  [476★], [262★], [279★], [200★], [202★], [111★], [79★]:

$${}^{(n)}\mathcal{E}_j = \sum_{l=0}^{\infty} V_{m,l} \frac{\mathcal{N}_l}{\mathcal{N}_m} {}^{(n)}c_{j-1,l}$$

$${}^{(n)}c_{j,k} = \frac{1}{\mathcal{E}_k^{(0)} - \mathcal{E}_n^{(0)}} \left( \sum_{l=1}^{j-1} {}^{(n)}\mathcal{E}_l {}^{(n)}c_{j-l,k} + \sum_{l=0}^{\infty} V_{k,l} \frac{\mathcal{N}_l}{\mathcal{N}_k} {}^{(n)}c_{j-1,l} \right).$$

Here  $V_{k,l} = \langle \psi_k^{(0)} | \hat{V} | \psi_l^{(0)} \rangle$  and the perturbed eigenfunctions  $\psi_n^{(g)}$  are normalized according to  $\langle \psi_n^{(g)} | \psi_n^{(0)} \rangle = \mathcal{N}_n$ . (For matrix formulations, see [115★], [80★].)

For the eigenvalue problem  $-\psi_n''(z) + (z^2 + z^4)\psi_n(z) = \mathcal{E}_n \psi_n(z)$  (mixed harmonic-quartic oscillator [61★], [63★], [62★], [179★]) one conveniently chooses the harmonic oscillator part as the unperturbed (and exactly solvable) part and  $(gz^4)|_{g=1}$  as the perturbation.

$$\hat{L}_0 = -\frac{\partial^2}{\partial z^2} + z^2.$$

$$\hat{V} = z^4.$$

$$\langle \psi_k^{(0)} | \hat{V} | \psi_l^{(0)} \rangle = \int_{-\infty}^{\infty} \psi_k(z) z^4 \psi_l(z) dz.$$

Because for each  $l$ , only finitely many of the  $V_{k,l} = \langle \phi_k | z^4 | \phi_l \rangle$  (where  $\phi_k(z)$  are the harmonic oscillator eigenfunctions) are nonvanishing, it is possible to calculate the sums in  ${}^{(n)}\mathcal{E}_j$  and  ${}^{(n)}c_{j,k}$  exactly for all  $n$  and  $j$ . Calculate the first few  ${}^{(n)}\mathcal{E}_j$  and the first few hundred  ${}^{(0)}\mathcal{E}_j$ . Is the exact calculation of  ${}^{(0)}\mathcal{E}_{1000}$  feasible?

Asymptotically, the  ${}^{(0)}\mathcal{E}_j$  have the form [61★], [527★], [337★], [121★], [548★], [333★], [523★]

$${}^{(0)}\mathcal{E}_j = -(-1)^j \frac{2\sqrt{6}}{\pi^{3/2}} \left(\frac{3}{2}\right)^j \left(j - \frac{1}{2}\right)! \left(1 + \frac{\alpha_1}{j} + \frac{\alpha_2}{j^2} + \frac{\alpha_3}{j^3} + \dots\right).$$

Conjecture exact values for  $\alpha_1$ ,  $\alpha_2$ , and  $\alpha_3$ .

For the mixed harmonic-quartic oscillator, the sum  $\sum_{j=0}^{\infty} 1^j {}^{(0)}\mathcal{E}_j$  is divergent [182★]. Given a (divergent) power series  $\sum_{j=0}^{\infty} a_j x^j$ , the diagonal Padé approximation of order  $M$  [524★], [39★], [517★], [47★], [38★], [328★], [546★]

$$p_{(M,M)}(x) = \frac{\begin{pmatrix} a_1 & a_2 & \cdots & a_M & a_{M+1} \\ a_2 & a_3 & \cdots & a_{M+1} & a_{M+2} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ a_M & a_{M+1} & \cdots & a_{2M-1} & a_{2M} \\ \sum_{k=M}^M a_{k-M} x^k & \sum_{k=M-1}^M a_{k-M+1} x^k & \cdots & \sum_{k=2}^M a_k x^k & \sum_{k=0}^M a_k x^k \end{pmatrix}}{\begin{pmatrix} a_1 & a_2 & \cdots & a_M & a_{M+1} \\ a_2 & a_3 & \cdots & a_{M+1} & a_{M+2} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ a_M & a_{M+1} & \cdots & a_{2M-1} & a_{2M} \\ x^M & x^{M-1} & \cdots & x & 1 \end{pmatrix}}$$

allows calculating finite approximate values of such series by using the first  $M$  coefficients  $a_j$ . Use the diagonal Padé approximation to calculate the ground-state energy  $\varepsilon_0^{(1)}$  to 10 correct digits.

b) Similar to the last subexercise, we consider again the problem  $(\hat{L}_0 + g \hat{V}) \psi_n(g; z) = \varepsilon_n(g) \psi_n(g; z)$ . The  $g$ -dependent quantities  $\varepsilon_n(g)$  and  $V_{k,l}(g) = \langle \psi_k(g) | \hat{V} | \psi_l(g) \rangle$  obey the following system of coupled differential equations [430★], [263★], [453★], [537★], [269★]:

$$\frac{\partial \varepsilon_n(g)}{\partial g} = V_{n,n}^{(g)}$$

$$\frac{\partial V_{k,l}(g)}{\partial g} = \sum_{j \neq k} \frac{V_{k,j}(g) V_{j,l}(g)}{\varepsilon_k(g) - \varepsilon_j(g)} + \sum_{j \neq l} \frac{V_{k,j}(g) V_{j,l}(g)}{\varepsilon_l(g) - \varepsilon_j(g)}.$$

Use this system to calculate the ground-state energy of the quartic oscillator to 10 digits by using  $\hat{L}_0 = -\frac{\partial^2}{\partial z^2} + z^2$ . and  $\hat{V} = (z^4 - z^2)$ .

## 11. L<sup>2</sup> Sextic Oscillator, Time-Dependent Calogero Potential

a) Use expansion in eigenfunctions of the harmonic oscillator to make an animation of the time-development of the following initial value problem as a function of  $\mathcal{K}$

$$i \frac{\partial \Psi(x, t)}{\partial t} = -\frac{\partial^2 \Psi(x, t)}{\partial x^2} + x^6 \Psi(x, t)$$

$$\Psi(x, 0) = e^{i\mathcal{K}x} \cos^2\left(\frac{\pi x}{4}\right) \theta(4 - x^2).$$

Let  $\mathcal{K}$  range from 0 to 6 and  $0 \leq t \leq 8$ . How does this expansion compare with a direct numerical solution of the initial value problem using `NDSolve`?

b) Use expansion in eigenfunctions of the Calogero potential to make an animation of the time-development of the following initial value problem as a function of  $\mathcal{K}$

$$i \frac{\partial \Psi(x, t)}{\partial t} = -\frac{\partial^2 \Psi(x, t)}{\partial x^2} + \left(x^2 + \frac{\gamma}{x^2}\right) \Psi(x, t)$$

$$\Psi(x, 0) = \theta(x - \pi) \theta(2\pi - x) \cos(\mathcal{K}(x - \pi)) \sqrt{\sin(x - \pi)}.$$

(For the special properties of the Calogero potential, see [123★].)

Let  $3 \leq \mathcal{K} \leq 12$ ,  $\gamma = 2$ , and  $0 \leq t \leq 2$ . The time-independent Schrödinger equation with the Calogero potential [215★], [27★], [573★], [250★], [196★], [408★], [428★], [350★], [138★], [576★], [575★], [197★]

$$-\frac{\partial^2 \psi_n(x)}{\partial x^2} + \left(x^2 + \frac{\gamma}{x^2}\right) \psi_n(x) = \varepsilon_n \psi_n(x)$$

has the following eigenvalues and (not normalized) eigenfunctions ( $\alpha = (4\gamma + 1)^{1/2} / 2$ ,  $\gamma > -1/4$ ):

$$\begin{aligned} \varepsilon_n &= 4n + 2\alpha + 2 \\ \psi_n(x) &= x^{\frac{1}{2}(2\alpha+1)} e^{-\frac{x^2}{2}} L_n^\alpha(x^2). \end{aligned}$$

(For  $\gamma < -1/4$ , see [235★])

## CHAPTER 3

### Exercises

#### 1.<sup>L1</sup> Asymptotic Series, Carlitz Expansion, Contour Lines of the Gamma Function, Bessel Zeros, Asymptotic Expansion of Gamma Function Ratio, Integrals of Function Compositions, $W_{1+i}(1+i)$

a) Special functions are often developed in asymptotic series. Taylor series are convergent, but asymptotic series are not. Investigate the convergence behavior of the following asymptotic representation of the Bessel function of order 0:

$$J_0(z) \sim \frac{1}{\pi \sqrt{2\pi z}} \left( \sum_{k=0}^{\infty} e^{-i(z-\pi/4)} \frac{\Gamma(k + \frac{1}{2})^2}{(-2iz)^k k!} + \sum_{k=0}^{\infty} e^{i(z-\pi/4)} \frac{\Gamma(k + \frac{1}{2})^2}{(2iz)^k k!} \right)$$

and the Airy function  $\text{Ai}(z)$

$$\text{Ai}(z) \sim \frac{1}{2\sqrt{\pi}} \frac{1}{z^{1/4}} \exp\left(-\frac{2}{3} z^{2/3}\right) \sum_{k=0}^{\infty} (-1)^k \frac{\Gamma(3k + \frac{1}{2})}{54^k \Gamma(k) \Gamma(k+1)} \left(\frac{2}{3} z^{2/3}\right)^{-k} \quad |\arg(z)| < \pi$$

for some specific values of  $z$  in the complex  $z$ -plane. To calculate numerical values of asymptotic series, one best (not taking into account hyperrefinements) sums only the terms as long as they are decreasing [208★].

b) The asymptotic expansion of the Airy function  $\text{Ai}(z)$  at  $z = \infty$  can be written in the form [436★]

$$\text{Ai}(z) \sim \frac{1}{2\sqrt{\pi}} \frac{1}{z^{1/4}} \exp\left(-\frac{2}{3} z^{2/3}\right) \left(1 + \sum_{k=0}^{\infty} \frac{2}{3} \frac{a_{k+1}}{k+1} z^{3/2}\right).$$

Here the  $a_k(\zeta)$  are defined through the recursion

$$a_1(\zeta) = -\frac{5}{72} \frac{1}{\zeta}$$

$$a_{k+1}(\zeta) = \left(\frac{k-1}{k}\right) a_k(\zeta) + \frac{1}{2k} \frac{\partial a_k(\zeta)}{\partial \zeta} + \frac{5}{72k} \int_{-\infty}^{\zeta} \frac{a_{k+1}(z)}{z^2} dz.$$

Calculate the 8 leading terms (as a Laurent series in  $2/3 z^{3/2}$ ) of the first 1000  $a_k(\zeta)$ . How well do these terms approximate the exact values?

c) Verify by a series expansion in  $z$  the following relation [940★] to some low order in  $z$ :

$$\left(\frac{az}{2}\right)^\mu \left(\frac{bz}{2}\right)^\nu = \sum_{k=0}^{\infty} (\sigma_k - \sigma_{k-2}) J_{\mu+k}(az) J_{\nu+k}(bz)$$

$$\sigma_{-1} = \sigma_{-2} = 0$$

$$\sigma_k = \frac{\Gamma(\nu+k+1)\Gamma(\mu+1)}{k!} \left(\frac{a}{b}\right)^k {}_2F_1\left(-k, \mu+1; -\nu-k; \frac{b^2}{a^2}\right).$$

d) Make a picture of the lines where  $\operatorname{Re}(\Gamma(z)) = 0$  and  $\operatorname{Im}(\Gamma(z)) = 0$  in the complex  $z$ -plane.

e) Calculate the first few (in magnitude) real zeros  $\nu_n$  of  $J_\nu(2)$ . What is remarkable here?

f) Calculate the first four coefficients  $c_i(\alpha, \beta)$  of the following series expansion:

$$\frac{\Gamma(z+\alpha)}{\Gamma(z+\beta)} \sim z^{\alpha-\beta} \sum_{i=0}^{\infty} \frac{c_i(\alpha, \beta)}{z^i}, \text{ as } z \rightarrow \infty.$$

g) Find the real  $x^*$  such that the thousands partial sum  $f_{1000}(x)$  of  $\sin(x)$ , where  $f_n(x) = \sum_{i=0}^n (-1)^i x^{2i+1} / (2i+1)!$  deviates from  $\sin(x)$  by  $10^{-1000}$ .

h) At which dimension  $d$  are the volume  $V = \pi^{d/2} / \Gamma(d/2 + 1)$  and the surface area  $A = d \pi^{d/2} / \Gamma(d/2 + 1)$  of a  $d$ -dimensional unit sphere maximal [41★], [1297★], [36★]?

The probability density  $p_d(\rho)$  for the Euclidean distance  $\rho$  of two points chosen at random in a  $d$ -dimensional sphere of radius 1 is [1298★]

$$p_d(\rho) = \frac{2d \rho^{d-1}}{B\left(\frac{d}{2} + \frac{1}{2}, \frac{1}{2}\right)} \left( {}_2F_1\left(\frac{1}{2}, \frac{1}{2} - \frac{d}{2}; \frac{3}{2}; 1\right) - \frac{1}{2} \rho {}_2F_1\left(\frac{1}{2}, \frac{1}{2} - \frac{d}{2}; \frac{3}{2}; \frac{\rho^2}{4}\right) \right).$$

What is the limit  $\lim_{d \rightarrow \infty} p_d(\rho)$ ? What is the average distance between two points in the limit  $d \rightarrow \infty$ ?

i) A radial symmetric potential function  $V_d(|\mathbf{x} - \mathbf{y}|)$  in  $d$  dimensions can be decomposed à la Fefferman–de la Llave through [590★]

$$V_d(|\mathbf{x} - \mathbf{y}|) = \int_0^\infty \int_{\mathbb{R}^d} \chi_{r/2}(\mathbf{z} - \mathbf{y}) g_d(r) \chi_{r/2}(\mathbf{x} - \mathbf{z}) d\mathbf{z} dr.$$

Here  $\chi_r(x) = \theta(|\mathbf{x}| - r)$  is the characteristic function of a ball around  $\mathbf{x}$  of radius  $r$ . The function  $g(r)$  can be expressed through

$$g_d(r) = \frac{2(-1)^{d+1}}{\Gamma\left(\frac{d-1}{2}\right) (\pi r^2)^{\frac{d-1}{2}}} \int_r^\infty V^{(d+1)}(\rho) \rho (\rho^2 - r^2)^{\frac{d-3}{2}} d\rho$$

for smooth  $V(r)$  and the convolution integral over the two balls through

$$\int_{\mathbb{R}^d} \chi_r(\mathbf{z} - \mathbf{y}) \chi_r(\mathbf{x} - \mathbf{z}) d\mathbf{z} = \left(\frac{\pi}{4}\right)^{\frac{d-1}{2}} \frac{\theta(2r - |\mathbf{x} - \mathbf{y}|)}{\Gamma(\frac{d+1}{2})} \int_{|\mathbf{x}|}^{2r} (4r^2 - \xi^2)^{\frac{d-1}{2}} d\xi.$$

Calculate  $g_d(r)$  for some potentials  $V_d(|\mathbf{x} - \mathbf{y}|)$  and derive integration-free formulas for  $g_d(r)$  for  $d = 3, 5, 7$  for potentials that vanish sufficiently fast at infinity.

**j)** Calculate the value of the Bessel functions  $J_{10^{100}}(10^{100})$  to 1000 digits.  $J_\nu(z)$  for  $z \approx \nu$  and  $\nu \rightarrow \infty$  can be efficiently computed by Meissel's formula [1359★]:

$$J_\nu(z) \sim \frac{1}{3\pi} \sum_{m=0}^{\infty} \left(\frac{z}{6}\right)^{-\frac{m+1}{3}} B_m(z - \nu) \sin\left(\frac{m+1}{3}\pi\right) \Gamma\left(\frac{m+1}{3}\right)$$

$$B_m(\zeta) = 6^{-\frac{m+1}{3}} b_m(m)$$

$$b_n(m) = [w^n] \left\{ e^{\zeta w} \left( \frac{\sinh(w) - w}{w^3} \right)^{-(m+1)/3} \right\}.$$

Here,  $[z^n]\{f(z)\}$  denotes the  $n$ th coefficient in the Taylor expansion of  $f(z)$  around  $z = 0$ .

**k)** The first zero  $z_0^{(\nu)}$  of the Bessel function  $J_\nu(z)$  can be bounded by [580★], [709★], [685★]

$$\frac{1}{(\sigma_n^{(\nu)})^n} < (z_0^{(\nu)})^2 < \frac{\sigma_n^{(\nu)}}{\sigma_{n+1}^{(\nu)}}.$$

Here,  $\sigma_n^{(\nu)}$  is the Rayleigh sum  $\sigma_n^{(\nu)} = \sum_{k=1}^{\infty} (z_k^{(\nu)})^{-2n}$ . The Rayleigh sum  $\sigma_n^{(\nu)}$  obeys the following recurrence relation:

$$\sigma_n^{(\nu)} = \frac{1}{\nu + n} \sum_{k=1}^{n-1} \sigma_k^{(\nu)} \sigma_{n-k}^{(\nu)}$$

$$\sigma_1^{(\nu)} = \frac{1}{4(\nu + 1)}.$$

Use these formulas to calculate  $z_0^{(1)}$  to 100 digits. What is the maximal  $n$  needed? How fast can one calculate  $z_0^{(1)}$  to 100 digits using Rayleigh sums?

**l)** For all positive integers  $n$ , the number  $x$  defined implicitly by  $K(1 - x)/K(x) = \sqrt{n}$  is algebraic [41★], [192★], [1427★]. Use numerical techniques to find an exact algebraic  $x$  for  $n = 10$ .

**m)** Try to calculate all 13824 indefinite integrals of the functions  $f_1(f_2(f_3(x)))$ , where  $f_i$  is a trigonometric, hyperbolic, inverse trigonometric, or inverse hyperbolic function. How many of the doable triple integrals will contain special functions? Which special functions appear and how often?

**n)** The ProductLog function  $W_k(z)$  has the following integral representation ( $z \notin (-1/e, 0)$ ) [1197★], [1198★], [692★]:

$$W_k(z) = 1 + (\log(z) + 2\pi i k - 1) \exp\left(\frac{i}{2\pi} \int_0^\infty \log\left(\frac{(2k-1)\pi i + t - \log(t) + \log(z)}{(2k+1)\pi i + t - \log(t) + \log(z)}\right) \frac{1}{t+1} dt\right).$$

Use this formula to calculate  $W_{1+i}(1+i)$  to 20 digits.

**o)** The Gumbel probability distribution  $p(x)$  has the form ( $a > 0$ ) [578★], [299★], [986★]:

$$p(x) = c (\exp(b(x - \xi) - e^{b(x-\xi)}))^{-a}.$$

Find the values of the parameters  $b(a)$ ,  $c(a)$ , and  $\xi(a)$  such that  $p(x)$  is normalized to 1, has a mean of 0, and a second moment of 1.

p) Consider the command `Binomial[x, y]` as a function of two complex variables  $x$ , and  $y$ . What are the “correct” values of `Binomial[negativeInteger, anotherNegativeInteger]`?

q) Find a closed form description of the curves that separate the white and the black areas in the following graphic.

```
ContourPlot[Im[(x + I y)^(x + I y)], {x, -10, 10}, {y, -10, 10},
  PlotPoints -> 250, Contours -> {0}];
```

r) Let  $g_n$  be the geometric mean of all irreducible fractions from the unit interval with maximal denominator  $n$  [923★]:

$$g_n = \sqrt[n]{\frac{1}{n} \times \frac{2}{n} \times \cdots \times \frac{n}{n}}.$$

Calculate the limit of  $g_n$  as  $n$  tends to infinity and the first correction term.

Calculate the following infinite product (known as the Wallis product [1063★], [1064★]) and the first correction term.

$$\frac{2}{1} \frac{2}{3} \frac{4}{3} \frac{4}{5} \frac{6}{5} \frac{6}{7} \frac{8}{7} \frac{8}{9} \frac{10}{9} \frac{10}{11} \cdots.$$

Calculate the following limit and the first correction term for large  $n$ :

$$\lim_{n \rightarrow \infty} \frac{2^{4n+2}}{(n+1)^3} \frac{(n+1)!^4}{(2n+1)!^2}.$$

Calculate the following limit and the first correction term for large  $n$ :  $\lim_{n \rightarrow \infty} \sum_{k=1}^{n^2} n / (k^2 + n^2)$  [552★].

s) Consider the following generalization  $\Gamma_k(z)$  of the classical Gamma function  $\Gamma(z)$ :  $\Gamma_k(z) = k^{z/k-1} \Gamma(z/k)$  [409★]. Derive polynomial partial differential equations that are fulfilled by  $\Gamma_k(z)$ .

t) The generalized Bell numbers  $B_k(n)$  are defined by [65★], [339★]

$$\frac{\exp(\exp(\cdots(\exp(z))))}{k \exp^s} = \sum_{k=0}^{\infty} \frac{B_k(n)}{n!} z^k.$$

Show by explicit calculation for  $1 \leq m, n \leq 6$  that the following identity holds:

$$B_m(n+1) = \sum_{k_1, k_2, \dots, k_m=0}^{\infty} \delta_{\sum_{j=1}^m k_j, n} \frac{n!}{\prod_{j=1}^m k_j!} \prod_{j=1}^m B_j(k_j).$$

u) Predict if `1 - Erfc[666.666]` will be a machine number.

v) For factorially divergent sums, Borel summation means expressing the factorial function through its integral representation and then exchanging summation and integration:

$$\sum_{k=1}^{\infty} f(k) (a + bk)! = \sum_{k=1}^{\infty} f(k) \int_0^{\infty} e^{-t} t^{a+bk} dt \stackrel{B}{=} \int_0^{\infty} e^{-t} \left( \sum_{k=1}^{\infty} f(k) t^{a+bk} \right) dt$$

Sums of the form  $s_j = \sum_{k=1}^{\infty} (-3)^k k^{-j} (k-1/2)!$ ,  $k = 0, 1, \dots$  occur in the perturbation expansion of the quartic anharmonic oscillator [742★], [553★]. Calculate the first few of these sums. The summands of these sums decrease with increasing  $j$ , do the sums decrease too? Conjecture a closed form for  $\lim_{j \rightarrow \infty} s_j$ .

w) Calculate the normalized ground-state  $\psi_N(z)$  of the Hamiltonian [992★], [993★], [994★], [85★]

$$\hat{H} = -\frac{\partial^2}{\partial z^2} + V(z)$$

$$V(z) = \frac{\frac{19z^2}{4} - (\sqrt{5} - \frac{1}{2})}{(z^2 + 1)^2}.$$

Calculate  $z^*$ , such that  $V(z^*) = \psi_N(z^*)$ .

x) Consider the two integrals  $\int_{-X}^X H_1(x) H_{3/2}(x) \exp(-x^2/2) dx$  and  $\int_0^X L_1(x) L_{3/2}(x) e^{-x} dx$  involving Laguerre functions  $L_\nu(x)$  and Hermite functions  $H_\nu(x)$ . Find the leading terms of these integrals for large real  $X$ . Laguerre and Hermite functions are orthogonal for nonnegative integer indices. Does orthogonality still hold for these fractional indices?

y) Evaluate the following integral [1358★], [536★], [944★]:

$$\frac{1}{\pi^3} \int_0^\pi \int_0^\pi \int_0^\pi \frac{1}{1 - \cos(x) \cos(y) \cos(z)} dx dy dz.$$

z) The function  $L(z) = \text{Li}_2(z) + 1/2 \ln(z) \ln(1-z)$  fulfills the two identities  $L(z) + L(1-z) = \pi^2/6$  and  $L(z) = L(z/(z-1)) + L(z^2)/2$ . In addition, for special arguments identities like [841★]

$$6L\left(\frac{1}{3}\right) - L\left(\frac{1}{9}\right) = \frac{\pi^2}{3}$$

$$2L\left(2 \cos\left(\frac{3}{7}\pi\right)\right) + L\left(\left(2 \cos\left(\frac{3}{7}\pi\right)\right)^2\right) = \frac{4}{21} \pi^2$$

$$3L\left(\frac{1}{2 \cos(\frac{\pi}{9})}\right) + 3L\left(\left(\frac{1}{2 \cos(\frac{\pi}{9})}\right)^2\right) - L\left(\left(\frac{1}{2 \cos(\frac{\pi}{9})}\right)^3\right) = \frac{7}{18} \pi^2$$

hold.

Write a program that searches for (and finds) such identities.

## 2.L<sup>2</sup> Elliptic Integrals

The incomplete elliptic integral of the third kind is defined by the following integral representation:

$$\Pi(n; \phi | m) = \int_0^\phi \frac{1}{(1 - n \sin(\varphi)) \sqrt{1 - m \sin(\varphi)}} d\varphi.$$

a) Derive an inhomogeneous, linear, third-order differential equation for  $\frac{\partial \Pi(n; \phi | m)}{\partial m}$  [256★]. (The coefficients will be polynomials in  $n$  and  $m$ .)

b) Derive an inhomogeneous, linear, third-order differential equation for  $\frac{\partial \Pi(n; \phi | m)}{\partial n}$ . (The coefficients will again be polynomials in  $n$  and  $m$ .)

c) Starting from the integral representation, derive a nonlinear, third-order differential equation for  $\frac{\partial \Pi(n; \phi | m)}{\partial \phi}$ .

d) Calculate a “nice” result for the following integral:

$$\int_{(3-2\sqrt{3})/12}^{1/12} \sqrt{\frac{3-12x}{(12x-1)(48x^2-24x-1)}} dx.$$

e) Show that in the addition theorem for elliptic integrals of the first kind

$$\int_0^x \frac{1}{\sqrt{(1-\tau^2)(1-k\tau^2)}} d\tau + \int_0^y \frac{1}{\sqrt{(1-\tau^2)(1-k\tau^2)}} d\tau = \int_0^{z(x,y)} \frac{1}{\sqrt{(1-\tau^2)(1-k\tau^2)}} d\tau$$

the  $z$  on the right-hand side as a function of  $x$  and  $y$  fulfills [99★]

$$(k y^2 z^2 - 1)^2 x^4 - 2((k(y^2 + z^2 - 2) - 2) z^2 + 1) y^2 + z^2 x^2 + (y^2 - z^2)^2 = 0.$$

f) Determine the magnetic field of a circular current (also beyond the axis), and examine it graphically. Then, investigate the magnetic field of a Helmholtz coil [261★] in the neighborhood of a symmetry point. In which direction is the field more inhomogeneous: in the radial or in the perpendicular direction?

### 3. L<sup>2</sup> Weierstrass Function

a) Visualize the following two Weierstrass functions:

$$\wp\left(z; \frac{8}{3}, \frac{8}{3}\right) \quad \text{and} \quad \wp'\left(z; \frac{8}{3}, \frac{8}{3}\right)$$

in the complex  $z$ -plane. What is an appropriate  $z$ -domain? In *Mathematica*, the Weierstrass  $\wp(z; g_2, g_3)$  is `WeierstrassP[z, {g2, g3}]` and its derivative  $\wp'(z; g_2, g_3)$  (with respect to  $z$ ) is `WeierstrassPPrime[z, {g2, g3}]`.

b) Make a picture of the function  $\wp'(z; g_2, g_3)$  over the Riemann  $z$ -sphere. Use appropriate values for  $g_2$  and  $g_3$ .

c) The function  $\wp(z; g_2, g_3)$  has the following series expansion around  $z = 0$ :

$$\wp(z; g_2, g_3) = \frac{1}{z^2} + \frac{g_2}{20} z^2 + \frac{g_3}{28} z^4 + c_6 z^6 + c_8 z^8 + \dots$$

By using the differential equation of the Weierstrass function:

$$\wp'^2(z; g_2, g_3) = 4\wp^3(z; g_2, g_3) + g_2\wp'(z; g_2, g_3) + g_3$$

(where the derivative is with respect to  $z$ ), find the coefficients  $c_6$  to  $c_{20}$ .

d) The Weierstrass function  $\wp(u; g_2, g_3)$  fulfills the differential equation (differentiation with respect to  $u$ ):

$$\wp'(u; g_2, g_3)^2 = 4\wp(u; g_2, g_3)^3 - g_2\wp(u; g_2, g_3) - g_3.$$

In [3★], formula 18.4.1, the following addition theorem is given:

$$\wp(u+v; g_2, g_3) = \frac{1}{4} \left( \frac{\wp'(u; g_2, g_3) - \wp'(v; g_2, g_3)}{\wp(u; g_2, g_3) - \wp(v; g_2, g_3)} \right)^2 - \wp(u; g_2, g_3) - \wp(v; g_2, g_3).$$

Derive a polynomial form of the addition theorem  $p(\wp(u+v; g_2, g_3), \wp(u; g_2, g_3), \wp(v; g_2, g_3))$  (this means  $p(x, y, z)$  being a polynomial in  $x, y$ , and  $z$ , symmetric in  $y$  and  $z$ ) by eliminating the derivative terms. Derive the corresponding double argument formula that expresses  $\wp(2v; g_2, g_3)$  polynomially in  $\wp(v; g_2, g_3)$ .



e) In [3★] formula 18.4.2, the following addition theorem for the derivative of the Weierstrass function  $\wp'(u; g_2, g_3)$  is given:

$$\wp'(u + v; g_2, g_3) = -(\wp(u + v; g_2, g_3) (\wp'(u; g_2, g_3) - \wp'(v; g_2, g_3)) + \wp(u; g_2, g_3) \wp'(v; g_2, g_3) - \wp'(u; g_2, g_3) \wp(v; g_2, g_3)) / (\wp(u; g_2, g_3) - \wp(v; g_2, g_3)).$$

Derive a polynomial form of the addition theorem  $q(\wp'(u + v; g_2, g_3), \wp'(u; g_2, g_3), \wp'(v; g_2, g_3))$  (this means  $q(x, y, z)$  is a polynomial in  $x, y$ , and  $z$ , symmetric in  $y$  and  $z$ ) by eliminating the nondifferentiated terms. Derive the corresponding double argument formula that expresses  $\wp'(2v; g_2, g_3)$  polynomially in  $\wp'(v; g_2, g_3)$ .

f) The general solution of the functional equation (Sutherland–Calogero model [263★], [1254★], [262★], [215★], [1318★], [789★], [255★], [217★])

$$\wp(x) \wp(y) + \wp(x) \wp(z) + \wp(y) \wp(z) = f(x) + f(y) + f(z)$$

for  $z = x + y$  is given by

$$\begin{aligned} \wp(x) &= \alpha \zeta(x; g_2, g_3) + \beta x \\ f(x) &= -\frac{1}{2} \left( \alpha^2 \zeta(x; g_2, g_3)^2 + \alpha^2 \frac{\partial \zeta(x; g_2, g_3)}{\partial x} + 2 \beta x \zeta(x; g_2, g_3) \alpha + \beta^2 x^2 \right) \\ \wp(x) \wp(y) + \wp(x) \wp(z) + \wp(y) \wp(z) &= f(x) + f(y) + f(z). \end{aligned}$$

Here,  $\zeta(x; g_2, g_3)$  is the Weierstrass Zeta function (in *Mathematica*, `WeierstrassZeta[x, {g2, g3}]`):

$$\zeta(x; g_2, g_3) = \frac{1}{x} + \int_0^x \left( \frac{1}{x^2} - \wp(x; g_2, g_3) \right) dx \quad \text{or} \quad \frac{\partial \zeta(x; g_2, g_3)}{\partial x} = -\wp(x; g_2, g_3).$$

Use the above addition formula for  $\wp(u + v; g_2, g_3)$  to show that  $\wp(x)$  and  $f(x)$  fulfill the above functional equation.

g) Use the above addition formula for  $\wp(u + v; g_2, g_3)$  to show that the following identity holds for  $z = x + y$  [413★]:

$$\zeta(x; g_2, g_3) + \zeta(y; g_2, g_3) + \zeta(z; g_2, g_3) = \sqrt{\wp(x; g_2, g_3) + \wp(y; g_2, g_3) + \wp(z; g_2, g_3)}.$$

h) The  $n$ -argument multiplication formula for Weierstrass function can be expressed in the following form ( $n \in \mathbb{N}$ ) [498★], [1042★], [499★]:

$$\begin{aligned} \wp(nz; g_2, g_3) &= \wp(z; g_2, g_3) - \frac{\psi_{n-1} \psi_{n+1}}{\psi_n^2} \\ \psi_1 &= 1 \\ \psi_2 &= -\wp'(z; g_2, g_3) \\ \psi_3 &= 3 \wp(z; g_2, g_3)^4 - \frac{3}{2} g_2 \wp(z; g_2, g_3)^2 - 3 g_3 \wp(z; g_2, g_3) - \frac{g_2^2}{16} \\ \psi_4 &= \wp'(z; g_2, g_3) \left( -2 \wp(z; g_2, g_3)^6 + \frac{5 g_2}{2} \wp(z; g_2, g_3)^4 + 10 g_3 \wp(z; g_2, g_3)^3 + \right. \\ &\quad \left. \frac{5 g_2^2}{8} \wp(z; g_2, g_3)^2 + \frac{g_2 g_3}{2} \wp(z; g_2, g_3) - \frac{g_2^3}{32} + g_3^2 \right) \\ \psi_n &= \begin{cases} -\psi_{\frac{n}{2}} \left( \psi_{\frac{n}{2}+2} \psi_{\frac{n}{2}-1}^2 - \psi_{\frac{n}{2}-2} \psi_{\frac{n}{2}+1}^2 \right) / \wp'(z; g_2, g_3) & \text{if } n \text{ is even} \\ \psi_{\frac{n-1}{2}+2} \psi_{\frac{n-1}{2}}^3 - \psi_{\frac{n-1}{2}-1} \psi_{\frac{n-1}{2}}^3 & \text{if } n \text{ is odd.} \end{cases} \end{aligned}$$

Use this formula to derive  $\wp(5v; g_2, g_3) = R(\wp(v; g_2, g_3))$ , where  $R$  is a rational function.

i) Show that the function  $\psi_\lambda(x)$  [758★], [1137★], [756★], [222★], [22★], [529★], [1018★]

$$\psi_\lambda(x) = \frac{\sigma(\lambda - x; g_2, g_3)}{\sigma(x; g_2, g_3) \sigma(\lambda; g_2, g_3)} e^{x\zeta(\lambda; g_2, g_3)}$$

is a solution of the Lamé equation [1352★], [1249★]:

$$-\psi_\lambda''(x) + 2\wp(x; g_2, g_3)\psi_\lambda(x) = -\wp(\lambda; g_2, g_3)\psi_\lambda(x).$$

Here  $\sigma(x; g_2, g_3)$  is the Weierstrass sigma function (in *Mathematica* `WeierstrassSigma[z, {g2, g3}]]`):

$$\sigma(x; g_2, g_3) = \exp\left(\int_0^x \left(\zeta(x; g_2, g_3) - \frac{1}{x}\right) dx\right) \quad \text{or} \quad \frac{\partial \sigma(x; g_2, g_3)}{\partial x} = \sigma(x; g_2, g_3) \zeta(x; g_2, g_3).$$

j) Visualize the Riemann surface of the inverse Weierstrass function  $\wp^{(-1)}(z; 1+i, 1-2i)$ .

k) The Weierstrass sigma function  $\sigma(z; g_2, g_3)$  fulfills a partial differential equation of the form

$$\frac{\partial^2 \sigma(z; g_2, g_3)}{\partial z^2} = G_2(z, g_2, g_3) \frac{\partial \sigma(z; g_2, g_3)}{\partial g_2} + G_3(z, g_2, g_3) \frac{\partial \sigma(z; g_2, g_3)}{\partial g_3} + G_C(z, g_2, g_3) \sigma(z; g_2, g_3).$$

The functions  $G_2(z, g_2, g_3)$ ,  $G_3(z, g_2, g_3)$ , and  $G_C(z, g_2, g_3)$  are total degree two polynomials of  $g_2$ ,  $g_3$ , and  $z$ . Use the series representation:

$$\sigma(z; g_2, g_3) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} a_{m,n} \frac{\left(\frac{g_2}{2}\right)^m (2g_3)^n}{(4m+6n+1)!} z^{4m+6n+1}$$

$$a_{0,0} = 1$$

$$a_{m,n} = \frac{16}{3} (n+1) a_{m-2,n+1} - \frac{1}{3} (2m+3n-1)(4m+6n-1) a_{m-1,n} + 3(m+1) a_{m+1,n-1} \quad \text{if } n, m \geq 0$$

$$a_{m,n} = 0 \quad \text{else}$$

to find the polynomials  $G_2$ ,  $G_3$ , and  $G_C$ .

l) The function

$$\Sigma(\tau) = \frac{\sigma\left(\frac{2}{3}\tau; g_2(\omega_1(1, \tau), \omega_2(1, \tau)), g_3(\omega_1(1, \tau), \omega_2(1, \tau))\right)^5}{\left(\sigma\left(\frac{1}{3}\tau; g_2(\omega_1(1, \tau), \omega_2(1, \tau)), g_3(\omega_1(1, \tau), \omega_2(1, \tau))\right)^4 \sigma\left(\frac{4}{3}\tau; g_2(\omega_1(1, \tau), \omega_2(1, \tau)), g_3(\omega_1(1, \tau), \omega_2(1, \tau))\right)\right)}$$

takes on algebraic values for certain  $\tau = i\sqrt{n}$ ,  $n \in \mathbb{N}$  [699★]. Conjecture at least 10 such values for  $\tau$  and express the corresponding values  $\Sigma(\tau)$  in radicals.  $(\{\omega_1(g_2, g_3), \omega_2(g_2, g_3)\})$  are the half periods corresponding to the invariants  $\{g_2, g_3\}$ . (In *Mathematica*, the half periods can be calculated from the invariants by the function `WeierstrassHalfPeriods[{g2, g3}]`.)

m) The equations of motions for a 2D periodic set of  $n$  point vertices  $z_\alpha(t)$  of strength  $\Gamma_\alpha$  ( $\alpha = 1, \dots, n$ ) are [210★], [1247★], [1024★], [1248★]

$$\frac{dz_\alpha(t)}{dt} = \frac{i}{2\pi} \sum_{\substack{\beta=1 \\ \alpha \neq \beta}}^n \Gamma_\beta \overline{\phi(z_\alpha(t) - z_\beta(t))}$$

$$\phi(z) = \zeta(z; g_2, g_3) + \left( \frac{\pi}{4|\operatorname{Im}(\omega_1 \bar{\omega}_2)|} - \frac{\zeta(\omega_1; g_2, g_3)}{\omega_1} \right) z - \frac{\pi}{4|\operatorname{Im}(\omega_1 \bar{\omega}_2)|} z.$$

(For 1D periodic point vertices, see [925★])

The basic lattice vectors are  $2\omega_1$  and  $2\omega_2$ ,  $\zeta(z; g_2, g_3)$  is the Weierstrass Zeta function and  $g_2, g_3$  are the invariants corresponding to the half periods  $\omega_1$  and  $\omega_2$ . Calculate and visualize orbits of a few vortices.

#### 4.<sup>L2</sup> Jacobi's Elliptic Functions

a) The Jacobi elliptic functions  $\operatorname{sn}(u|m)$ ,  $\operatorname{sd}(u|m)$ ,  $\operatorname{sc}(u|m)$ ,  $\operatorname{nd}(u|m)$ ,  $\operatorname{nc}(u|m)$ ,  $\operatorname{dn}(u|m)$ ,  $\operatorname{dc}(u|m)$ ,  $\operatorname{cn}(u|m)$ ,  $\operatorname{cd}(u|m)$ ,  $\operatorname{cd}(u|m)$ ,  $\operatorname{ds}(u|m)$ , and  $\operatorname{ns}(u|m)$  fulfill nonlinear ordinary differential equations of the following type (where  $pq$  in the following formulas is any of the just-mentioned 12 Jacobi functions):

$$\frac{\partial}{\partial z} pq(u|m) = \pm \sqrt{a_{pq}(m) + b_{pq}(m) pq^2(u|m) + c_{pq}(m) pq^4(u|m)}$$

$$\frac{\partial^2}{\partial z^2} pq(u|m) = d_{pq}(m) pq(u|m) + e_{pq}(m) pq^3(u|m).$$

By using the built-in capabilities of *Mathematica* to give series approximations of the Jacobi elliptic function, determine the coefficients  $a_{pq}(m)$ ,  $b_{pq}(m)$ ,  $c_{pq}(m)$ ,  $d_{pq}(m)$ , and  $e_{pq}(m)$  for all of the above elliptic Jacobi functions.

b) The 12 Jacobi functions  $\operatorname{cd}(u|m)$ ,  $\operatorname{cn}(u|m)$ ,  $\operatorname{cs}(u|m)$ ,  $\operatorname{dc}(u|m)$ ,  $\operatorname{dn}(u|m)$ ,  $\operatorname{ds}(u|m)$ ,  $\operatorname{nc}(u|m)$ ,  $\operatorname{nd}(u|m)$ ,  $\operatorname{ns}(u|m)$ ,  $\operatorname{sc}(u|m)$ ,  $\operatorname{sd}(u|m)$ , and  $\operatorname{sn}(u|m)$  satisfy many identities similar to the ones known for trigonometric functions. The equivalent formulas to  $\sin^2(x) + \cos^2(x) = 1$  are

$$\operatorname{cn}(u|m)^2 + \operatorname{sn}(u|m)^2 = 1,$$

$$\operatorname{dn}(u|m)^2 + m \operatorname{sn}(u|m)^2 = 1.$$

Derive all possible formulas for pairs of squares of Jacobi functions  $pq(u|m)$  and  $rs(u|m)$  of the form

$$f(m) pq(u|m)^2 + g(m) rs(u|m)^2 + h(m) pq(u|m)^2 rs(u|m)^2 + l(m) = 0$$

where  $f, g, h$ , and  $l$  are constant or linear polynomials in  $m$ .

c) The Jacobi functions  $pq(u|m)$  have polynomial addition formulas  $p(pq(u+v|m), pq(u|m), pq(v|m), m) = 0$  where  $p$  is a polynomial.

The typically shown formulas are [3★]:

$$\operatorname{sn}(u+v|m) = \frac{\operatorname{cn}(v|m) \operatorname{dn}(v|m) \operatorname{sn}(u|m) + \operatorname{cn}(u|m) \operatorname{dn}(u|m) \operatorname{sn}(v|m)}{1 - m \operatorname{sn}(u|m)^2 \operatorname{sn}(v|m)^2}$$

$$\operatorname{cn}(u+v|m) = \frac{\operatorname{cn}(u|m) \operatorname{cn}(v|m) - \operatorname{sn}(u|m) \operatorname{dn}(u|m) \operatorname{sn}(v|m) \operatorname{dn}(v|m)}{1 - m \operatorname{sn}(u|m)^2 \operatorname{sn}(v|m)^2}$$

$$\operatorname{dn}(u+v|m) = \frac{\operatorname{dn}(u|m) \operatorname{dn}(v|m) - m \operatorname{sn}(u|m) \operatorname{cn}(u|m) \operatorname{sn}(v|m) \operatorname{cn}(v|m)}{1 - m \operatorname{sn}(u|m)^2 \operatorname{sn}(v|m)^2}.$$

Using the defining formulas for Jacobi functions, the above square identities, and these three addition formulas, derive the addition formulas expressed only in  $\text{pq}(u | m)$ . This means as  $p(\text{pq}(u + v | m), \text{pq}(u | m), \text{pq}(v | m), m) = 0$  for all twelve Jacobi functions.

**d)** Use the following implicit definition of the Jacobi function  $\text{sn}(z | m)$  to derive the first five terms of the series expansion of  $\text{sn}(z | m) = \sum_{n=0}^{\infty} c_n(z) m^n$  around  $m = 0$  [984★]:

$$z = \int_0^{\text{sn}(z|m)} \frac{1}{\sqrt{1-t^2} \sqrt{1-mt^2}} dt.$$

An alternative way to calculate this series expansion is given by the following set of formulas [1386★]:

$$\text{sn}(z | m) = \sum_{n=0}^{\infty} \frac{m^n}{(2n)!} f_{2n}(z)$$

$$f_0(z) = \sin(z)$$

$$g_{2n}(z) = \sum_{k=0}^n \binom{2n}{2k} f_{2k}(z) f_{2n-2k}(z)$$

$$g_{2n}''(z) = -4 g_{2n}(z) - 8n(2n-1) g_{2n-2}(z) + 12(2n-1)n \sum_{k=0}^{n-1} \binom{2n-2}{2k} g_{2k}(z) g_{2n-2k-2}(z)$$

$$g_{2n}(0) = g_{2n}'(0) = 0$$

$$g_0(z) = \sin(z)^2.$$

Use these formulas to calculate the  $f_2(z)$ ,  $f_4(z)$ ,  $f_6(z)$ , and  $f_8(z)$  and compare with the above result.

**e)** The Jacobi elliptic function  $\text{sn}$  obeys the following functional equation.

$$\text{sn}(z | m) = - \frac{2 \left( m \text{sn}\left(\frac{z}{4} | m\right)^4 - 2 \text{sn}\left(\frac{z}{4} | m\right)^2 + 1 \right) \left( m \left( \text{sn}\left(\frac{z}{4} | m\right)^2 - 2 \right) \text{sn}\left(\frac{z}{4} | m\right)^2 + 1 \right) \text{sn}\left(\frac{z}{2} | m\right)}{\left( m \text{sn}\left(\frac{z}{4} | m\right)^4 - 1 \right)^2 \left( m \text{sn}\left(\frac{z}{2} | m\right)^4 - 1 \right)}.$$

Use this equation to calculate  $\text{sn}(1 + i | 1/3 + 2i)$  to 100 digits.

**f)** Polynomial (and rational) functions (with  $z$ -independent coefficients) of the Jacobi functions  $\text{cn}(z | m)$ ,  $\text{sn}(z | m)$ , and  $\text{dn}(z | m)$  are frequently solutions of a Sturm–Liouville-type eigenvalue equation of the form

$$-\Psi''(m | z) + V(m | \Psi(m | z)) \Psi(m | z) = \varepsilon(m) \Psi(m | z)$$

where the potential  $V$  is a function of  $z$  only through  $\Psi(m | z)$ . Find some  $\Psi(m | z)$  where the corresponding  $V(m | \Psi(m | z))$  is a rational function of  $\Psi(m | z)$  and  $m$  with no explicit  $z$ -dependence.

**g)** Find a solution of the form

$$u(x, t) = \sum_{j=0}^o \alpha_j(k, c, m; \beta_1, \beta_2, \beta_3) \text{sn}(k(x - ct) | m)^j$$

of the nonlinear wave equation (Bussinesq equation) [831★], [1350★]

$$\frac{\partial^2 u(x, t)}{\partial t^2} = \beta_1 \frac{\partial^2 u(x, t)}{\partial x^2} + \beta_2 \frac{\partial^4 u(x, t)}{\partial x^4} + \beta_3 \frac{\partial^2 u(x, t)^2}{\partial x^2}.$$

Find some other nonlinear evolution equations of the form  $\psi_t = p(\psi, \psi_x, \psi_{xx}, \psi_{xxx}, \dots)$  or  $\psi_{tt} = q(\psi, \psi_x, \psi_{xx}, \psi_{xxx}, \dots)$  or  $\psi_{ttt} = \dots$  where  $p, q, \dots$  are polynomials and the equations have solutions that can be expressed as a sum of powers of  $\text{sn}(k(x - ct) | m)$  [1121★], [343★], [1041★], [1390★], [90★], [308★], [470★], [1391★], [1402★], [635★], [1185★], [1392★], [1393★], [829★], [830★], [1351★], [819★].

h) Derive a second-order differential equation of the function  $w(z) = \text{sn}(a \log(a + bz) | m)$ ; view  $a$  and  $b$  as integration constants [265★].

i) Solve the equation for a pendulum  $\varphi''(t) = -\sin(\varphi(t))$ ,  $\varphi(0) = 0$ ,  $0 \leq \varphi_0 \leq \pi$ ,  $\varphi'(0) = 2 \sin(\varphi_0/2)$  [46★] numerically along straight rays in the complex  $t$ -plane ( $\varphi_0$  is the maximal elongation). Explain the resulting “complex oscillations” using visualizations of the Riemann surface of the solution

$$\varphi(t) = 2 \arcsin\left(\sin\left(\frac{\varphi_0}{2}\right) \text{sn}\left(t \mid \sin^2\left(\frac{\varphi_0}{2}\right)\right)\right).$$

## 5.<sup>L2</sup> Rocket with Discrete Propulsion, Neat Product, Harmonic Oscillator Spectrum

a) The discrete rocket problem is as follows: Imagine a rocket that burns its fuel in discrete masses of size  $(m_i - m_f)/n$  (where  $m_i$  is the initial mass,  $m_f$  the final mass, and  $n$  is the number of burns) rather than continuously. Give an analytic formula for the final velocity as a function of  $n$ . What happens in the limiting case  $n \rightarrow \infty$ ?

b) Calculate a nice result for the following product [318★]. Find some generalizations that can be calculated in closed form.

$$\prod_{k=1}^{\infty} \exp\left(-\frac{1}{k}\right) \left(1 + \frac{1}{k} + \frac{1}{k^2}\right).$$

c) Using the functions `DSolve` and `Series`, calculate the eigenvalues  $\varepsilon_n = 2n + 1$ ,  $n \in \mathbb{N}$  of the harmonic oscillator [1381★], [1361★],  $-\psi_n''(z) + z^2 \psi_n(z) = \varepsilon_n \psi_n(z)$ ,  $z \in (-\infty, \infty)$ .

## 6.<sup>L2</sup> Contour Integral, Asymptotics of Bessel Function, Isophotes, Circular Andreev Billiard

a) The Bessel function  $J_\nu(z)$  has the following integral representation [1359★]:

$$J_\nu(z) = \frac{\Gamma(\frac{1}{2} - \nu) (\frac{z}{2})^{2\nu}}{2\pi i \sqrt{\pi}} \int_C e^{izt} (t^2 - 1)^{\nu - \frac{1}{2}} dt.$$

A possible parametrization of the contour  $C$  in the complex  $t$ -plane is given by  $t(\varphi) = a \cos(\varphi) + i b \sin(2\varphi)$ ,  $a > 1$ ,  $b > 0$ ,  $0 \leq \varphi \leq 2\pi$ . The contour  $C$  is located on the Riemann surface of the (generically multivalued) integrand. Implement this representation, and use it to calculate the numerical value of  $J_\nu(i\pi)$ .

b) Bessel functions of large real positive order  $\nu$  and arguments  $z < \nu$  can be expanded in an asymptotic series in the following way [1359★], [316★]: We start from the differential equation for  $J_\nu(\nu z)$  with respect to  $z$

$$z^2 \frac{d^2 J_\nu(\nu z)}{d z^2} + z \frac{d J_\nu(\nu z)}{d z} + \nu^2 (z^2 - 1) J_\nu(\nu z) = 0$$

and introduce new (in the moment unknown) functions  $u_i(z)$  via

$$J_\nu(z) = \frac{\nu^\nu}{\Gamma(\nu+1)} \exp(u(z))$$

$$u(z) = \nu \int_c^z u_1(\zeta) d\zeta + \sum_{i=-\infty}^0 \nu^i \int_0^z u_i(\zeta) d\zeta.$$

The constant  $c$  is chosen in such a way that for small  $z$ , this expansion agrees with the ordinary series expansion of  $J_\nu(z)$  around  $z = 0$ . The functions  $u_i(z)$  have to be calculated by equating the coefficients of the powers of  $\nu$  to zero. Calculate symbolically the first terms of this series expansion, and use the resulting series to calculate the numerical value of  $J_{1000}(100)$ .

c) The intensity  $I_\nu(u)$  of a converging spherical wave, which was diffracted at a circular aperture, is in the meridional plane given by the square of the absolute value of the following integral

$$I_\nu(u) = \int_0^1 \rho J_0(\nu \rho) e^{-i u \rho^2/2} d\rho$$

[824★], [188★], [1239★], [891★]. Visualize the intensity  $I_\nu(u)$  inside the domain  $|u| < 10\pi$ ,  $|\nu| < 5\pi$ .

d) The eigenfunctions superconductor–normal metal system is described by the Bogoliubov–de Gennes equation (a generalization of the Schrödinger equation) [391★], [1209★], [5★], [119★], [1171★], [1182★]

$$\begin{pmatrix} -\hbar^2/2 m(\mathbf{r})^{-1} \Delta + V(\mathbf{r}) - \mu(\mathbf{r}) & \delta(\mathbf{r}) \\ \overline{\delta(\mathbf{r})} & -\hbar^2/2 m(\mathbf{r})^{-1} \Delta + V(\mathbf{r}) - \mu(\mathbf{r}) \end{pmatrix} \begin{pmatrix} \psi_n^{(e)}(\mathbf{r}) \\ \psi_n^{(h)}(\mathbf{r}) \end{pmatrix} = \varepsilon_n \begin{pmatrix} \psi_n^{(e)}(\mathbf{r}) \\ \psi_n^{(h)}(\mathbf{r}) \end{pmatrix}.$$

Here the quantities  $m(\mathbf{r})$ ,  $V(\mathbf{r})$ ,  $\mu(\mathbf{r})$ , and  $\delta(\mathbf{r})$  are the position-dependent mass, potential, chemical potential, and pair potential (which vanishes in the nonsuperconducting state).  $u_n(\mathbf{r})$  and  $v_n(\mathbf{r})$  are the electron and hole components of the wave function and  $\varepsilon_n$  are the eigenvalues. For the case of a concentric superconductor–normal conductor arrangement with equal chemical potentials, no (interface) potential, and no mass mismatch, a superconductor of diameter  $\rho^{(S)}$  and normal conductor of diameter  $\rho^{(N)}$  the problem simplifies considerably. (Here we assume the superconductor in the center surrounded by the normal conductor, meaning  $\rho^{(S)} < \rho^{(N)}$ .)

After separation of variables and matching wave functions, the eigenvalue problem reduces to [357★] finding the roots of the following determinantal equation

$$\begin{vmatrix} \psi_m^{(N,e)}(\varepsilon, \rho^{(S)}) & 0 & \delta^{(e)}(\varepsilon) \psi_m^{(S,e)}(\varepsilon, \rho^{(S)}) & \delta^{(h)}(\varepsilon) \psi_m^{(S,h)}(\varepsilon, \rho^{(S)}) \\ 0 & \psi_m^{(N,h)}(\varepsilon, \rho^{(S)}) & \psi_m^{(S,e)}(\varepsilon, \rho^{(S)}) & \psi_m^{(S,h)}(\varepsilon, \rho^{(S)}) \\ \psi_m^{(N,e)'}(\varepsilon, \rho^{(S)}) & 0 & \delta^{(e)}(\varepsilon) \psi_m^{(S,e)'}(\varepsilon, \rho^{(S)}) & \delta^{(h)}(\varepsilon) \psi_m^{(S,h)'}(\varepsilon, \rho^{(S)}) \\ 0 & \psi_m^{(N,h)'}(\varepsilon, \rho^{(S)}) & \psi_m^{(S,e)'}(\varepsilon, \rho^{(S)}) & \psi_m^{(S,h)'}(\varepsilon, \rho^{(S)}) \end{vmatrix} = 0$$

where (choosing appropriate units) the electron wave function components are

$$\psi_m^{(N,e)}(\varepsilon, \rho^{(S)}) = J_m(k(\varepsilon) \rho^{(S)}) - J_m(k(\varepsilon) \rho^{(N)}) Y_m(k(\varepsilon) \rho^{(S)}) / Y_m(k(\varepsilon) \rho^{(N)})$$

$$\psi_m^{(S,e)}(\varepsilon, \rho^{(S)}) = J_m(q(\varepsilon) \rho^{(S)})$$

and the hole wave functions are  $\psi_m^{(N,h)} = \psi_m^{(N,e)}(-\varepsilon, \rho^{(S)})$  and  $\psi_m^{(S,h)} = \overline{\psi_m^{(S,e)}(-\varepsilon, \rho^{(S)})}$ . Here a prime denotes differentiation with respect to the second argument  $\rho^{(S)}$ . The azimuthal quantum number  $m$  is integer. The wave vectors  $k$  and  $q$  are  $k(\varepsilon) = (1 + \varepsilon)^{1/2}$  and  $q(\varepsilon) = (1 + (\varepsilon - \Delta_0)^{1/2})^{1/2}$ . Finally the electron and hole pairing potentials are  $\delta^{(e)}(\varepsilon) = \Delta_0(\varepsilon - (\varepsilon^2 - \Delta_0^2)^{-1/2})$  and  $\delta^{(h)}(\varepsilon) = \overline{\delta^{(e)}(\varepsilon)}$ .

The eigenvalues of the resulting determinant have interesting dependence on  $m$  [357★], [835★]. Visualize the eigenvalues for  $0 < \varepsilon_n < \Delta_0$  and  $0 \leq m \leq 2.5 \rho^{(S)}$  for the parameter values  $\Delta_0 = 0.15$ ,  $\rho^{(S)} = 200$ , and  $\rho^{(N)} = 400$ .

### 7.<sup>L1</sup> Euler's Integral for Beta Function, Beta Probability Distribution, Euler's Constant

a) The Beta function  $B(p, q)$  can be represented by the following integral (see [608★] and [278★]):

$$B(p, q) = -\frac{e^{i(q-p)}}{4 \sin(p\pi) \sin(q\pi)} \int_C t^{p-1} (1-t)^{q-1} dt.$$

Here,  $C$  is a contour that encloses the point  $\{0, 0\}$  and  $\{1, 0\}$  (see [795★], [753★], [623★], [765★], and [1382★]), in a way that is topologically equivalent to a path parametrized by:

$$\{x(s), y(s)\} = \{(\cos(s)^2 \cosh(\sin(\pi/4 + s))^2 - \sin(s)^2 \sinh(\sin(\pi/4 + s))^2), \\ \cos(s) \cos(\sin(\pi/4 + s)) \sin(s) \sin(\sin(\pi/4 + s))\}.$$

The integration has to be carried out on the Riemann surface of the integrand. (So the integrand is a continuous function along the path of integration.) Implement the numerical evaluation of the Beta function via the above integral representation.

b) Visualize a discrete realization of the probability density  $w(x) \propto (1-x^2)^\gamma$  using  $x_j(\gamma)$ ,  $0 \leq x_j(\gamma) \leq 1$ ,  $j = 0, \dots, n$  [1378★].

c) Euler's constant  $\gamma$  has the well-known representation  $\gamma = \lim_{n \rightarrow \infty} (\sum_{k=1}^n 1/k - \ln(n))$  [1401★], [404★], [403★]. Find a generalization of the form

$$\gamma = \lim_{n \rightarrow \infty} \left( \left( \sum_{k=1}^n 1/k \right) - \ln \left( n + \left( \sum_{j=0}^o \frac{\alpha_j}{n^j} \right) \right) \right)$$

that has optimal convergence properties for  $o = 100$ .

### 8.<sup>L2</sup> Time-Dependence in cos-Potential, Singular Potential Eigenvalues

a) Use expansion in eigenfunctions to visualize the time-development of the following initial value problem for a triple well potential

$$i \frac{\partial \Psi(x, t)}{\partial t} = -\frac{\partial^2 \Psi(x, t)}{\partial x^2} - V_0 \cos(x) \Psi(x, t) \\ \Psi(-3\pi, t) = \Psi(3\pi, t) \\ \Psi(x, 0) = \cos(\mathcal{K} x) \cos^2\left(\frac{\pi}{2} \frac{x}{x_M}\right) \theta(x_M^2 - x^2)$$

for  $-3\pi \leq x \leq 3\pi$ ,  $0 \leq t \leq 10$ . Use  $V_0 = 12$ ,  $\mathcal{K} = 6$ ,  $x_M = \pi/6$ . How does this expansion compare with a direct numerical solution of the initial value problem using `NDSolve`?

b) Calculate bound states for the potential  $V(x) = -e^x$  in the Schrödinger equation  $-\psi''(x) + V(x)\psi(x) = \varepsilon\psi(x)$  [506★], [725★], [668★], [39★]. Calculate the corresponding WKB eigenvalues.

### 9.<sup>L2</sup> Dependencies, Numerical Function Evaluation, Usage Messages, Derivative Definition

a) By looking at examples of mathematical functions, find out which functions are used in internal computations of those mathematical functions.

b) Find examples for functions and exact arguments such that the result of `N[specialFunction[arguments]]` is incorrect. (`N[specialFunction[arguments], precisionLargerThanMachinePrecision]` is, nearly always, correct).

c) Numeric functions (meaning functions that carry the `NumericFunction` attribute) have usage messages like `BesselJ[n, z]` gives the Bessel function "...". Check which other "kinds" of usage messages exist for numeric functions.

d) Assume you have a (special) function  $Y(z)$ , such that  $Y'(0) = c$ , but  $Y'(z)$  cannot be expressed in closed form for general  $z$ . How could one implement that `Y'[0]` evaluates, but avoid the constant presence of a definition for `Derivative`?

### 10.<sup>L3</sup> Perturbation Theory, Pendulum with Finite Mass Cord

a) Consider the following eigenvalue problem (where  $\lambda$  is the eigenvalue) [1140★], [846★], [479★], [59★]:

$$-y''(x) + \alpha x y(x) = \lambda y(x), \quad y(-l/2) = y(l/2) = 0.$$

For small  $\alpha$  ( $\alpha \ll \pi/l^2$ ), starting with the exact solution of the problem, determine the dependence of  $\lambda_i = \lambda_i(\alpha)$  on  $\alpha$  in the form:

$$\lambda_i(\alpha) \approx \lambda_i(\alpha = 0) + c_1 \alpha + c_2 \alpha^2.$$

b) Consider the following eigenvalue problem in  $(-\infty, \infty)$  for  $v_0 < 0$  (where  $\lambda$  is the continuous eigenvalue) [59★]:

$$-y''(x) + \theta \left( \left( \frac{l}{2} \right)^2 - x^2 \right) V_0 y(x) + \alpha x y(x) = \lambda y(x).$$

(In physics terms, we are considering a quantum well in an electric field in the limit of small electric fields.) Now, the spectrum is for finite  $\alpha$  a continuous one. For small  $\alpha$  ( $\alpha \rightarrow 0$ ), again starting with the exact solution of the problem, determine the dependence of the  $\lambda_i = \lambda_i(\alpha)$  on  $\alpha$  in the form

$$\lambda_i(\alpha) \approx \lambda_i(\alpha = 0) + c_1 \alpha + c_2 \alpha^2$$

where  $\lambda_i, \lambda_i < v_0$  (which means it is a Gamov or quasi-bound state [394★], [1002★], [181★]) is now defined as a solution of the "eigenvalue equation" (pole condition of the corresponding Green's function [6★], [1097★], [177★], and [770★]) which one obtains by taking into account only outgoing waves to the far left and only asymptotically vanishing solutions to the far right. Check the limit  $\alpha \rightarrow 0$  for the eigenvalue equation and the limit (calculated in part a)  $V_0 \rightarrow \infty$  for  $c_2$ .

c) The harmonic small-angle oscillations of a pendulum with a bob of mass  $M$  on a flexible string of mass  $m$  and uniform mass density are described by the following differential equation [56★], [934★]:

$$\left( \frac{lM}{m} + x \right) z''(x) + z'(x) + \frac{\omega^2}{g} z(x) = 0$$

Here  $l$  is the length of the string,  $g$  the acceleration due to gravity,  $\omega$  the angular frequency, and  $z(x)$  the parametrized form of the string. Here the  $x$ -axis runs horizontally and the  $z$ -axis upward. The string is fixed at  $x = z = 0$  and the bob moves along the  $x$ -axis. The boundary conditions are  $z(0) = 0$  and  $g z'(l) = -\omega^2 z(l)$ .

Calculate the lowest order corrections to the angular frequency due to the finite mass of the string  $\omega(m/M) = \omega_0 + c_1(m/M) + c_2(m/M)^2 + \dots$  where  $\omega_0 = (g/l)^{1/2}$ .

### 11.<sup>L2</sup> Fermi–Dirac Integrals, Sum of All Reciprocal 9-Free Numbers, Zagier's Function

a) In [1321★], the following approximation of the Fermi–Dirac integral

$$F_\alpha(z) = \frac{1}{\Gamma(1+\alpha)} \int_0^\infty \frac{t^\alpha}{1+z^{-1}e^t} dt$$



as

$$\begin{aligned}
 F_a^{(n,k)}(z) &\approx \frac{2\pi \csc(a\pi)}{\Gamma(a+1)} \sum_{i=0}^n (\pi^2 (2i+1)^2 + \log^2(z))^{a/2} \cos\left(a\left(\pi - \tan^{-1}\left(\frac{(2i+1)\pi}{\log(z)}\right)\right)\right) + \\
 &\frac{\pi}{\Gamma(a+1)} \cos\left(a\left(\pi - \tan^{-1}\left(\frac{(2(n+1)+1)\pi}{\log(z)}\right)\right)\right) \csc(a\pi) (\pi^2 (2(n+1)+1)^2 + \log^2(z))^{a/2} - \\
 &2 \csc(a\pi) (\pi^2 (2(n+1)+1)^2 + \log^2(z))^{\frac{a+1}{2}} \times \\
 &\left(\sum_{i=0}^k \frac{\zeta(2i)}{\Gamma(a+2(1-i))} (\pi^2 (2(n+1)+1)^2 + \log^2(z))^{-i} \sin\left(a\pi - (a-2i+1) \tan^{-1}\left(\frac{(2(n+1)+1)\pi}{\log(z)}\right)\right)\right)
 \end{aligned}$$

was given. Here  $1 < z < \infty$ ,  $-1 < \alpha < \infty$ ,  $\alpha \neq 0, 1, 2, \dots$ ,  $k = 0, 1, 2, \dots$ ,  $2k > a + 1$ ,  $n = 0, 1, \dots$  and  $\zeta(x)$  is the Riemann Zeta function.

For moderate values of  $k$  and  $n$  ( $n < 8$ ), examine the usability of this expression (accuracy and availability of all needed functions) for other programs.

**b)** The asymptotic expansion for  $\eta \rightarrow \infty$  of the integral (a slightly rewritten form of the integral from the last subexercise)

$$\mathcal{F}_d(\eta) = \frac{1}{\Gamma(d/2)} \int_0^\infty \frac{\varepsilon^{d/2-1}}{1 + e^{\varepsilon-\eta}} d\varepsilon$$

is for  $d \in \mathbb{N}$  given by [412★], [519★], [1146★]

$$\begin{aligned}
 \mathcal{F}_d(\eta) &\underset{\eta \rightarrow \infty}{=} \mathcal{F}_{d,o}^{(\text{alg})}(\eta) + \mathcal{F}_{d,o}^{(\text{exp})}(\eta) \\
 \mathcal{F}_{d,o}^{(\text{alg})}(\eta) &= \left( \sum_{k=0}^{\lfloor d/4 \rfloor} \frac{(2 - 2^{2-2k}) \zeta(2k)}{\Gamma(d/2 - 2k + 1)} \eta^{d/2-2k} \right) + \frac{\sin(d\pi/2)}{\pi} \sum_{k=\lfloor d/4 \rfloor + 1}^o \frac{(2 - 2^{2-2k}) \zeta(2k)}{\Gamma(2k - d/2)} \eta^{d/2-2k} \\
 \mathcal{F}_{d,o}^{(\text{exp})}(\eta) &= \cos(\pi(d/2 - 1)) \sum_{k=1}^o \frac{(-1)^{k+1}}{k^{d/2}} e^{-k\eta}.
 \end{aligned}$$

A graph of  $\mathcal{F}_{d,o}^{(\text{alg})}(\eta) / \mathcal{F}_{d,o}^{(\text{exp})}(\eta)$  in the  $d, \eta$ -plane shows for  $o \rightarrow \infty$  “special” points. Calculate the location of these points for  $d \rightarrow \infty$  to 20 digits.

**c)** The sum [684★], [653★], [838★]

$$s = \sum_{\substack{k=1 \\ k \text{ is } 9\text{-free}}}^\infty \frac{1}{k}$$

of all reciprocal numbers that are free of the digit 9 (in base 10) is a convergent sum. It is given by [485★], [78★]

$$s = \beta_0 \ln(10) + \sum_{k=2}^\infty 10^{-k} \beta(k-1) \zeta(k)$$

where the  $\beta_k$  are implicitly defined by:

$$\sum_{k=1}^n \binom{n}{k} (10^{-k+n+1} - 10^k + 1) \beta(n-k) = 10(11^n - 10^n), \quad n = 1, 2, \dots$$

Calculate a 50-digit approximation of  $s$ .

d) Consider the “special” function  $\varphi(z)$  defined as [1409★], [43★]:

$$\varphi(z) = \sum_{n=0}^{\infty} \prod_{k=1}^n (1 - z^k).$$

For  $z = \exp(2\pi i p/q)$ ,  $p, q \in \mathbb{Z}$ ,  $q \neq 0$ , the sum converges; for all other complex values of  $z$ , the sum diverges. Up to which denominators  $q$  can one use machine arithmetic to calculate  $\varphi(z)$ ? As a function of  $q$ , the relation  $\langle |\varphi(z)| \rangle \propto q^\alpha$  holds for large  $q$  (averaging  $\langle \cdot \rangle$  is with respect to  $p$ ). Find an approximative value of  $\alpha$ . Visualize for some  $p/q$  how the sum converges as one adds terms.

## 12.<sup>L2</sup> Heat Equation, Green’s Function for a Rectangle, Theta Function Addition Formulas, Theta Function Series Expansion, Bose Gas

a) Find the solution of the following boundary-value problem [116★]

$$\begin{aligned} \frac{\partial}{\partial t} T(x, t) &= a^2 \frac{\partial^2}{\partial x^2} T(x, t) \\ T(0, t) &= T(l, t) = 0 \\ T(x, 0) &= \delta(x - y) \end{aligned}$$

using elliptic Theta functions:

$$\vartheta_3(u, q) = 1 + 2 \sum_{n=1}^{\infty} q^{n^2} \cos(2n u)$$

where  $\vartheta_3(u, q) = \text{EllipticTheta}[3, u, q]$ . Examine graphically the dependence on temperature.

b) The Green’s function [430★], [1268★] for the Laplace equation with homogeneous Dirichlet boundary conditions on a rectangle  $(0, a) \times (0, b)$  usually is written in the form:

$$G_{ab}(x, y, x', y') = \frac{4}{ab\pi^2} \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \frac{\sin(\frac{m\pi x}{a}) \sin(\frac{n\pi y}{b}) \sin(\frac{m\pi x'}{a}) \sin(\frac{n\pi y'}{b})}{(\frac{m}{a})^2 + (\frac{n}{b})^2}.$$

(Sometimes, it is also written in the form of a single sum as a Fourier expansion in  $\sin(n\pi x/a) \sin(n\pi x'/a)$  [105★], [483★], [658★].)

Using elliptic Theta functions, it is possible to find a closed form for this sum (see, e.g., [1006★], [1271★], [659★], and [350★]):

$$G_{ab}(x, y, x', y') = \frac{1}{2\pi} \operatorname{Re} \left( \ln \left( \frac{\vartheta_1\left(\frac{\pi(z+z')}{2a}, q\right) \vartheta_1\left(\frac{\pi(z-z')}{2a}, q\right)}{\vartheta_1\left(\frac{\pi(z+z')}{2a}, q\right) \vartheta_1\left(\frac{\pi(z-z')}{2a}, q\right)} \right) \right)$$

with  $q = e^{-\pi b/a}$ ,  $z = x + iy$ ,  $z' = x' + iy'$ . Here,  $\vartheta_1(z, q)$  is the Theta function  $\text{EllipticTheta}[1, z, q]$ .

As a Green’s function of a 2D problem,  $G_{ab}(x, y, x', y')$  must have the following three properties:

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)G_{ab}(x, y, x', y') = -\frac{1}{\pi^2} \delta(x-x') \delta(y-y')$$

$$G_{ab}(x, y, x', y') = -\frac{1}{2\pi} \ln \sqrt{(x-x')^2 + (y-y')^2} + \text{smoothFunction}(x, y, x', y')$$

$$G_{ab}(x, y, x', y') = 0 \quad \text{for } \{x, y\} \text{ on the boundary of the rectangle.}$$

Can one establish symbolically these three properties directly using *Mathematica*? Examine graphically whether the boundary values are 0, whether a logarithmic singularity is present at  $z = z'$ , and whether the minimax principle holds (i.e.,  $G_{ab}(x, y, x', y')$  has no local minima or maxima in the interior).

Given the Green's function, the solution of the boundary value problem

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\psi(x, y) = 0$$

$$\psi(x, y)|_{\{x, y\} \in \partial R_{a,b}} = u(x, y)$$

(where  $\partial R_{a,b}$  is the boundary of the rectangle) can be expressed as [1336★], [1416★]

$$\psi(x, y) = - \int_{\partial R_{a,b}} \frac{\partial G_{ab}(x, y, x', y')}{\partial \vec{n}'} u(x', y') ds'$$

Here  $\partial \cdot / \partial \vec{n}'$  is the outward directed normal derivative with respect to the primed variables and  $ds'$  is the arc length measure and the integration extends along the boundary of the rectangle  $\partial R_{a,b}$ .

Use this representation to numerically solve the boundary value problem

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\psi(x, y) = 0$$

$$\psi(0, y) = \psi(2, y) = 1$$

$$\psi(x, 0) = \psi(x, 4) = 2$$

in the rectangle  $R = (0, 2) \times (0, 1)$  and to visualize the solution.

c) The Theta functions  $\vartheta_k(z, q)$  (in *Mathematica* `EllipticTheta[k, z, q]`),  $k \in \{1, 2, 3, 4\}$ ,  $z \in \mathbb{C}$ ,  $q \in \mathbb{C}$ ,  $|q| < 1$ ) fulfill many identities. One class of identities are addition formulas of the form [792★], [862★], [755★], [175★], [1093★], [1236★]

$$\vartheta_{i_1}(w, q) \vartheta_{i_2}(x, q) \vartheta_{i_3}(y, q) \vartheta_{i_4}(z, q) \pm \vartheta_{j_1}(w, q) \vartheta_{j_2}(x, q) \vartheta_{j_3}(y, q) \vartheta_{j_4}(z, q) =$$

$$\pm \vartheta_{k_1}(\omega, q) \vartheta_{k_2}(\xi, q) \vartheta_{k_3}(\psi, q) \vartheta_{k_4}(\zeta, q) \pm \vartheta_{l_1}(\omega, q) \vartheta_{l_2}(\xi, q) \vartheta_{l_3}(\psi, q) \vartheta_{l_4}(\zeta, q)$$

where

$$\omega = (w + x + y + z)/2$$

$$\xi = (w + x - y - z)/2$$

$$\psi = (w - x + y - z)/2$$

$$\zeta = (w - x - y + z)/2$$

and  $i_1, i_2, i_3, i_4, j_1, j_2, j_3, j_4, k_1, k_2, k_3, k_4, l_1, l_2, l_3, l_4 \in \{1, 2, 3, 4\}$ . Use numerical techniques to find all identities of the above form. Calculate a “generating” set of identities.

d) Consider the Theta function  $\vartheta_3(z, q)$  (in *Mathematica*, it is `EllipticTheta[3, z, q]`)

$$\vartheta_3(z, q) = 1 + 2 \sum_{k=1}^{\infty} q^{k^2} \cos(kz).$$

Use the partial differential equation for  $\vartheta_3(z, q)$

$$-\frac{1}{4} \frac{\partial^2 \vartheta_3(z, q)}{\partial z^2} = q \frac{\partial \vartheta_3(z, q)}{\partial q}$$

to derive the first eight terms in the series expansion of  $\vartheta_3(z, q)$ . Use the ordinary differential equation for  $\vartheta_3(q) = \vartheta_3(0, q)$  [1428★], [980★], [1396★]

$$\begin{aligned} &(\vartheta_3(q)^2 (d^3 \vartheta_3(q)) - 15 \vartheta_3(q) (d\vartheta_3(q)) (d^2 \vartheta_3(q)) + 30 (d\vartheta_3(q))^3)^2 + \\ &32 (\vartheta_3(q) (d^2 \vartheta_3(q)) - 3 (d^2 \vartheta_3(q))^2)^3 - \vartheta_3(q)^{10} (\vartheta_3(q) (d^2 \vartheta_3(q)) - 3 (d^2 \vartheta_3(q))^2)^2 = 0 \end{aligned}$$

(here,  $d = q \frac{\partial}{\partial q}$  was used for brevity) to express these coefficients  $c_0(q), \dots, c_{10}(q)$  as functions of  $\vartheta_3(q), \vartheta_3'(q)$ , and  $\vartheta_3''(q)$ .

e) The canonical partition function for  $N$  identical noninteracting bosons can be expressed as  $Z_N(\beta) = N^{-1} \sum_{n=1}^N Z_1(n\beta) Z_{N-n}(\beta)$  [1167★], [189★], [961★], [87★], [1168★], [786★], [444★]. Here  $Z_0 = 1$ ,  $\beta = 1/(k_B T)$  and  $Z_1(\beta)$  is the one-particle partition function. For a particle in a 3D box of dimensions  $L \times L \times L$  with infinite walls, the one-particle partition function is [1166★], [583★], [360★], [939★], [398★], [491★], [1251★], [283★]

$$Z_1^{(\text{box})}(\beta) = \left( \sum_{v=1}^{\infty} e^{-x v^2} \right)^3 = \left( \frac{1}{2} (\vartheta_3(0, e^{-x}) - 1) \right)^3 = \left( \sqrt{\frac{2}{2\pi}} K(q^{-1}(e^{-x})) - \frac{1}{2} \right)^3$$

where  $x = \beta \varepsilon_v$ ,  $\varepsilon_v = \hbar^2 / (2m) (\pi n/L)^2$  (or  $x = 3/8 (\lambda(T)/L)^2$ ,  $\lambda(T) = h(3m k_B T)^{-1/2}$  with  $\lambda(T)$  the de Broglie thermal wavelength),  $K(z)$  being the complete elliptic integral of the first kind, and  $q^{-1}(z)$  the inverse nome (in *Mathematica* `InverseEllipticNomeQ`). The ground state has energy  $3 \varepsilon_v$ .

The corresponding result for a 3D harmonic oscillator with identical frequencies is [231★], [687★], [847★], [1166★], [368★], [444★], [707★]  $Z_1^{(\text{HO})}(\beta) = (\sum_{v=1}^{\infty} e^{-\tilde{x}(v+1/2)})^3 = (e^{\tilde{x}/2} / (e^{\tilde{x}} - 1))^3$  where  $\tilde{x} = \beta \tilde{\varepsilon}_v$ ,  $\tilde{\varepsilon}_v = \hbar \omega$ . The ground state has energy  $3/2 \tilde{\varepsilon}_v$ .

The probability that  $n$  out of  $N$  particles occupy the state  $\varepsilon$  at temperature  $T$  is [1363★], [243★], [1166★], [1285★], [1056★]

$$P_{\varepsilon}^{(N)}(n; T) = \frac{1}{Z_N(\beta)} (e^{-n\beta\varepsilon} Z_{N-n}(\beta) - e^{-(n+1)\beta\varepsilon} Z_{N-n-1}(\beta)).$$

Visualize the average ground-state occupation for  $N = 100$  for various temperatures for the 3D box and the harmonic oscillator.

The mean energy of  $N$  particles is  $U_N(T) = k_B T^2 (\partial \ln(Z_N(\beta)) / \partial T)_{N,L}$  and the specific heat  $c_{v,N}(T) = 1/N \partial U_N(T) / \partial T$ . Visualize  $c_{v,N}(T)$  for various temperatures and particle numbers  $N$  for the 3D box and the harmonic oscillator.

### 13.<sup>L3</sup> Scattering on Cylinder, Coulomb Scattering, Spiral Waves, Optical Black Hole, Corrugated Wall Scattering, Random Solutions of the Helmholtz Equation

a) The scattered wave  $\mathcal{E}(r, \varphi; t)$  of an incoming plane electromagnetic wave  $E \exp(i\omega t + ikx)$ , scattered on a conducting cylinder of radius  $R$  and potential zero, is given by [798★], [1300★], [826★], [666★], [826★]:

$$\mathcal{E}(r, \varphi; t) = -E \left( \frac{J_0(kR)}{H_0^{(2)}(kR)} H_0^{(2)}(kr) + 2 \sum_{n=1}^{\infty} (-i)^n \frac{J_n(kR)}{H_n^{(2)}(kR)} H_n^{(2)}(kr) \cos(n\varphi) \right).$$

Here,  $H_0^{(2)}(x)$  is the Hankel function of the second kind,  $H_0^{(2)}(x) = J_n(x) - i Y_n(x)$ . Visualize the scattering process.

**b)** Water waves (Poincaré waves) in constant depth water are governed by the 2D Helmholtz equation with the boundary conditions  $\mathbf{n} \cdot \text{grad } u(\mathbf{r}) + i \beta \mathbf{t} \cdot \text{grad } u(\mathbf{r})$  on scatterers ( $\mathbf{t}$  is the normalized tangent vector and  $\mathbf{n}$  is the normalized normal vector). The solution of the scattering problem of a disk is [886★]

$$u(r, \varphi; t) = u_0 \left( e^{i k x} - \sum_{n=-\infty}^{\infty} i^n \frac{n R J'_n(k R) - n \beta J_n(k R)}{n R H_0^{(1)'}(k R) - n \beta H_0^{(1)}(k R)} H_n^{(1)}(k r) e^{i n \varphi} \right).$$

Here,  $H_0^{(1)}(x)$  is the Hankel function of the first kind,  $H_0^{(1)}(x) = J_n(x) + i Y_n(x)$  and primes denote differentiation with respect to the argument. Visualize this scattering process for various  $\beta$  (the parameter taking into account the rotation of the earth).

**c)** The scattering of a vertically polarized electromagnetic wave  $\mathcal{E}_z(r, \varphi) e^{i \omega t}$  impinging from the left on an infinite dielectric cylinder of radius  $R$  and refractive index  $n$  can be described by the following equations [1414★], [1177★], [609★]:

$$\mathcal{E}_z(r, \varphi) = \begin{cases} \mathcal{E}_0 \sum_{m=-\infty}^{\infty} a_m J_m(k r) e^{i m \varphi} & \text{for } r \leq R \\ \mathcal{E}_0 e^{i k x} + \mathcal{E}_0 \sum_{m=-\infty}^{\infty} b_m H_m^{(1)}(k r) e^{i m \varphi} & \text{for } r \geq R \end{cases}$$

$$a_m = i^m \frac{J'_m(k R) H_0^{(1)}(k R) - J_m(k R) H_0^{(1)'}(k R)}{n J'_m(n k R) H_0^{(1)}(k R) - J_m(n k R) H_0^{(1)'}(k R)}$$

$$b_m = i^m \frac{J'_m(k R) J_m(n k R) - J_m(k R) J'_m(n k R)}{n J'_m(n k R) H_0^{(1)}(k R) - J_m(n k R) H_0^{(1)'}(k R)}.$$

Here  $\mathcal{E}_0$  is the amplitude of the incoming wave,  $k$  is the wave vector ( $k = 2 \pi / \lambda$ ),  $n$  is the index of refraction, and  $H_m^{(1)}(z)$  is again the Hankel function of the first kind.

Make an animation showing  $|\mathcal{E}_z(r, \varphi)|$  for a cylinder with radius  $R \approx 10^1 \lambda$  with the index of refraction varying from frame to frame.

**d)** The quantum-mechanical wavefunction for the scattering process of an asymptotically plane wave  $\psi(\mathbf{r}) \sim e^{i k z}$  as  $|\mathbf{r}| \rightarrow \infty$  (unavoidable logarithmic terms suppressed) on a Coulomb potential  $V(r) \sim \kappa / r$  is given by the following series [1302★], [785★], [988★], [340★], [17★], [1267★], [730★], [821★], [107★]:

$$\psi(r, \vartheta) = \sum_{l=0}^{\infty} (2l + 1) i^l e^{i \eta_l(\kappa; k)} R_l(\kappa; k r) P_l(\cos(\vartheta))$$

$$\eta_l(\kappa; k) = \text{Arg}(\Gamma(l + i \kappa / k + 1))$$

$$R_l(\kappa; k r) = \frac{e^{-\frac{\pi \kappa}{2k}} (2 k r)^l}{(2 l + 1)!} e^{i k r} |\Gamma(l + i \kappa / k + 1)| {}_1F_1(l + i \kappa / k + 1; 2 l + 2; -2 i k r).$$

(For the corresponding formula in  $d$  dimensions, see [1388★].) Here  $\eta_l(\kappa; k)$  is the phase shift. It contains the Gamma function  $\Gamma(z)$  and the Legendre polynomials  $P_l(z)$ . Negative  $\kappa$  correspond to attracting potentials and positive  $\kappa$  correspond to repulsive potentials. Generate an animation that shows how  $\text{Re}(\psi(\mathbf{r}))$  and  $|\psi(\mathbf{r})|^2$  behave as a function of the potential strength  $\kappa$ .

**e)** Make a circular contour plot of the real or the imaginary part of the function  $u_n(r, \varphi)$ :

$$u_n(r, \varphi) = e^{i n \varphi} J_n(\sqrt{\mu} r).$$

Here,  $0 \leq \varphi \leq 2\pi$ ,  $0 \leq r \leq R$  ( $R \approx 25$  is a suitable value),  $n = 1, 2, 3, \dots$ , and  $\mu$  (in general a complex quantity) is determined by the following equation:

$$\sqrt{\mu} J_{n-1}(\sqrt{\mu} R) - n\left(\frac{1}{R} + i\right) J_n(\sqrt{\mu} R) = 0.$$

The resulting pictures visualize spiral waves of scalar reaction-diffusion equations. (For details, see [397★].)

**f)** The behavior of a light wave (impinging from the right) near a vortex can be approximately described by [810★], [811★]

$$F(\nu; r, \varphi; t) = \sum_{m=-\infty}^{\infty} \phi_m(\nu; r, \varphi) e^{i\omega t}$$

$$\phi_m(\nu; r, \varphi) = (-i)^{\sqrt{m^2+2\nu m}} J_{\sqrt{m^2+2\nu m}}(kr) e^{im\varphi}.$$

Here  $k$  is the wave vector and  $\omega$  the frequency of the light wave.  $\nu$  is the strength of the vortex. Make an animation that shows how the light wave bends around the vortex with increasing vortex strength  $\nu$ .

**g)** The following equations describe the stationary 2D scattering problem of a plane wave (with wave vector  $\mathbf{k}$  and angle  $\alpha$  to the  $y$ -axis) on the periodic curve  $y = b \sin(\beta x)$  with Dirichlet boundary conditions:

$$-\frac{\partial^2}{\partial x^2} \psi_{k,\alpha}(x, y) - \frac{\partial^2}{\partial y^2} \psi_{k,\alpha}(x, y) = k^2 \psi_{k,\alpha}(x, y)$$

$$\psi_{k,\alpha}(x, b \sin(\beta x)) = 0$$

Expanding  $\psi_{k,\alpha}(x, y)$  in Bragg-reflected waves gives [1319★], [1405★], [1252★], [1357★], [924★], [1356★], [995★], [825★], [666★], [661★], [1313★], [73★], [168★], [20★]

$$\psi_{k,\alpha}(x, y) = e^{i(k_x x + k_y y)} + \sum_{j=-\infty}^{\infty} c_j(k, \alpha) e^{i(K_x^{(j)} x + K_y^{(j)} y)}.$$

Here the abbreviations  $k_x = k \sin(\alpha)$ ,  $k_y = k \cos(\alpha)$ ,  $K_x^{(j)} = k_x + j\beta$ , and  $K_y^{(j)} = ((k_x^2 + k_y^2) - K_x^{(j)2})^{1/2}$  were used.

The  $c_j(k, \alpha)$  are solutions of the following infinite system of linear equations:

$$J_n(b k_y) + \sum_{j=-\infty}^{\infty} c_j(k, \alpha) J_{n-j}(b K_y^{(j)}) = 0.$$

Make an animation that shows the  $|\psi_{k,\alpha}(x, y)|$ ,  $\text{Re}(\psi_{k,\alpha}(x, y)) = 0$ , and  $\text{Im}(\psi_{k,\alpha}(x, y)) = 0$  as a function of  $k$  and  $\alpha$ .

**h)** Make an animation of contour plots of  $\text{Re}(\psi_\tau(r, \varphi)) = 0$  and  $\text{Im}(\psi_\tau(r, \varphi)) = 0$  where

$$\psi_\tau(r, \varphi; k) = \sum_{n=-\infty}^{\infty} c_n(\tau) e^{in\varphi} J_n(kr)$$

is a random superposition of orthogonal solutions of the 2D Helmholtz equation  $\Delta\psi = k^2\psi$  [176★], [143★], [167★], [1143★], [941★].

Here  $r$  and  $\varphi$  are polar coordinates,  $k$  is a real constant, and the  $c_n(\tau)$  are smooth random functions of  $\tau$ .

Make 3D contour plots of the corresponding 3D functions

$$\psi(r, \vartheta, \varphi; k) = \sum_{l=0}^{\infty} \sum_{m=-l}^l c_{l,m} \frac{J_{l+1/2}(kr)}{\sqrt{kr}} Y_{lm}(\vartheta, \varphi)$$

where the  $Y_{lm}(\vartheta, \varphi)$  are spherical harmonics and the  $c_{l,m}$  are again random coefficients.

**14.<sup>L1</sup> Wronskian of Legendre Functions, Separation of Variables in Toroidal Coordinate System**

a) Prove that the Wronskian for the Legendre functions is given by:

$$\begin{aligned} W(P_\nu^\mu(z), Q_\nu^\mu(z)) &= P_\nu^\mu(z) \frac{\partial Q_\nu^\mu(z)}{\partial z} - Q_\nu^\mu(z) \frac{\partial P_\nu^\mu(z)}{\partial z} \\ &= \frac{\Gamma(\nu + \mu + 1)}{\Gamma(\nu - \mu + 1)} \frac{1}{1 - z^2}. \end{aligned}$$

b) The relationship between toroidal coordinates [945★] and Cartesian ones is given by:

$$\{x, y, z\} = \left\{ \frac{c \sinh(\eta) \cos(\vartheta)}{\cosh(\eta) - \cos(\varphi)}, \frac{c \sinh(\eta) \sin(\vartheta)}{\cosh(\eta) - \cos(\varphi)}, \frac{c \sin(\varphi)}{\cosh(\eta) - \cos(\varphi)} \right\}.$$

Visualize the coordinate surfaces of the toroidal coordinate system.

Show that the Laplace equation can be solved by the method of separation of variables in toroidal coordinates and that the solution is a linear combination of functions of the form

$$\sqrt{2(\cosh(\eta) - \cos(\varphi))} (c_1 \cos(\varphi) + c_2 \sin(\varphi)) (c_3 \cos(\vartheta) + c_4 \sin(\vartheta)) (c_5 P_\nu^\mu(\cosh(\eta)) + c_6 Q_\nu^\mu(\cosh(\eta)))$$

where the  $c_i$  are constants to be determined by the specific boundary conditions. Use the package `Calculus`VectorAnalysis``. For some application of the use of toroidal coordinates for the solution of electromagnetic boundary value and other problems, see [645★], [122★], [109★], [983★], [9★], [10★], [1320★], [279★], and [806★].

**15.<sup>L2</sup> Riemann–Siegel Formula, Zeros of Hurwitz Zeta Function, Zeta Zeta Function, Harmonic Polylogarithms,  $1 \times 2 \times 3 \times \dots = \sqrt{2\pi}$**

a) The Riemann Zeta function  $\zeta(z) = \sum_{k=1}^{\infty} k^{-z}$ ,  $\text{Re}(z) > 1$  is of most interest along the critical line  $z = 1/2 + it$  [794★], [445★], [657★], [1280★], [1036★], [148★], [149★], [321★], [86★]. There, it can be conveniently written as  $\zeta(1/2 + it) = Z(t) e^{i\vartheta(t)}$ . Here,  $\vartheta(t)$  is the Riemann–Siegel Theta function (in *Mathematica* `RiemannSiegelTheta[t]`) and  $Z(t)$  is the Riemann–Siegel function (in *Mathematica* `RiemannSiegelZ[t]`).  $Z(t)$  is purely real for real  $t$ . The Riemann–Siegel Theta function can be expressed through the logarithm of the Gamma function (in *Mathematica*, `LogGamma[z]`):

$$\vartheta(t) = \text{Im} \left( \log \Gamma \left( i \frac{t}{2} + \frac{1}{4} \right) - \frac{t}{2} \log(t) \right).$$

For large positive  $t$ , the Riemann–Siegel function  $Z(t)$  has the following expansion (this is the celebrated asymptotic Riemann–Siegel formula):

$$Z(t) \underset{t \rightarrow \infty}{\sim} 2 \sum_{k=1}^{\nu(t)} \frac{1}{\sqrt{k}} \cos(\vartheta(t) - t \log(k)) + R(t)$$

where  $\nu(t) = \lfloor (t/(2\pi))^{1/2} \rfloor$ .

The term  $R(t)$  can be expanded in powers of  $t^{1/4}$  [445★], [1211★]:

$$R(t) = (-1)^{\nu(t)-1} \left(\frac{t}{2\pi}\right)^{-\frac{1}{4}} \sum_{k=0}^{\infty} c_k \left(\sqrt{\frac{t}{2\pi}} - \nu(t)\right) \left(\frac{t}{2\pi}\right)^{-\frac{k}{2}}.$$

The coefficients  $c_k(p)$  can be expressed in the following way:

$$c_k(p) = [\omega^k] \left[ \exp\left(i\left(\log\left(\frac{t}{2\pi}\right) - \frac{t}{2} - \frac{\pi}{8} - \vartheta(t)\right)\right) \times [y^0] \left( \left( \sum_{j=0}^{\infty} A_j(y) \omega^j \right) \left( \sum_{j=0}^{\infty} \psi^{(j)}(p) \frac{y^j}{j!} \right) \right) \right].$$

In the last formula,  $[x^n](f(x))$  denotes the coefficient of  $x^n$  of the Taylor series expansion of  $f(x)$  around  $x = 0$ . The sequence  $A_j(y)$  obeys the following recursion relation:

$$A_j(y) = -\frac{1}{2} y A_{j-1}(y) - \frac{1}{32\pi^2} \frac{\partial^2}{\partial y^2} \frac{A_{j-1}(y)}{y}$$

$$A_0(y) = e^{2\pi i y^2}.$$

Finally,  $\psi(p)$  is the following function:

$$\psi(p) = \frac{\cos(2\pi(p^2 - p - 1/16))}{\cos(2\pi p)}.$$

Calculate the first 10 coefficients  $c_k$ . Taking in  $R(t)$  the first 10 terms into account, how many correct digits does one get for  $t = 10^6$ ? (For more efficient ways to calculate the  $c_k$ 's, see [149★].)

b) The generalized Zeta function (Hurwitz's Zeta function [783★], [1231★])  $\zeta(z, \alpha)$  is defined in *Mathematica* by the analytic continuation of the following formula (when  $\alpha$  not a negative integer or 0):

$$\zeta(z, \alpha) = \sum_{n=0}^{\infty} \frac{1}{((n + \alpha)^2)^{z/2}}.$$

The *Mathematica* form is `Zeta[z, α]`. For  $\alpha = 1$ , the function  $\zeta(z, 1)$  is Riemann's  $\zeta(z)$  function with all its nontrivial zeros (conjectured) on the line  $z = 1/2 + it$ ,  $t > 0$  (see [445★] and [657★]). Visualize the dependence of the zeros of  $\zeta(z, \alpha)$  for  $1/2 \leq \alpha \leq 1$  [502★].

c) For positive integers  $s$ , the values of the Zeta function  $Z(s)$  (of the nontrivial zeros  $z_k = 1/2 + it_k$ ) of the Riemann Zeta function  $\zeta(z)$  [804★]

$$Z(s) = \sum_{k=1}^{\infty} \frac{1}{\left(\frac{1}{4} + t_k\right)^s}$$

(here conjugate roots have been grouped pairwise so that  $t_k > 0$  is assumed) can be obtained in closed form by equating coefficients of  $s^n$  in the following identity [1341★], [1342★], [335★], [1343★]:

$$\sum_{k=1}^{\infty} \frac{Z(k)}{k} (s(1-s))^k = -\left( \left( \log(2\sqrt{\pi}) + \frac{\gamma}{2} - 1 \right) s + \sum_{k=2}^{\infty} \frac{((1-2^{-k})\zeta(k) - 1)}{k} s^k - \sum_{l=1}^{\infty} \frac{1}{l} \left( \sum_{k=1}^{\infty} \frac{\gamma_{k-1}}{(k-1)!} s^k \right)^l \right).$$

Here  $\gamma_k$  are the Stieltjes constants (in *Mathematica* `StieltjesGamma[k]`). Calculate the exact values for  $Z(1)$ , ...,  $Z(5)$  and compare the values with the ones obtained by summing over the first 1000 nontrivial zeros explicitly.



d) The harmonic polylogarithm functions  $H(a_1, a_2, \dots, a_n; z)$  are defined recursively through [1101★], [526★], [937★], [527★], [172★], [1217★], [378★], [1338★]

$$H(a_1, a_2, \dots, a_n; z) = \int_0^z f(a_1; \zeta) H(a_2, \dots, a_n; \zeta) d\zeta$$

$$f(-1, z) = 1/(1+z) \quad H(-1; z) = +\ln(1+z)$$

$$f(\pm 0, z) = 1/z \quad H(\pm 0; z) = +\ln(z)$$

$$f(-1, z) = 1/(1-z) \quad H(+1; z) = -\ln(1-z).$$

For which  $a_k = -1, 0, 1$  can *Mathematica* find exact finite values of  $H(a_1, a_2; 1)$ ,  $H(a_1, a_2, a_3; 1)$ , and  $H(a_1, a_2, a_3, a_4; 1)$ ?

e) Sums (especially infinite sums) whose summands contain special functions can often be calculated by using an integral representation for the special function, then interchanging summation and integration (assuming the conditions to do this are fulfilled) [1233★], [874★]. Use the integral representation

$$\psi^{(n)}(z) = \frac{\partial^n}{\partial t^n} \left( \gamma + \int_0^1 \frac{1-t^{z-1}}{1-t} dt \right)$$

for the  $n$ th derivative of the Digamma function  $\psi(z)$  to calculate some sums of the form [1011★], [1012★], [1013★]

$$\sum_{k=1}^{\infty} R(k) P(\psi(z), \psi^{(1)}(z), \dots).$$

Here  $R(k)$  is a rational function in  $k$  and  $P(x, y, \dots)$  is a polynomial. Can one calculate some sums that the built-in `Sum` cannot find?

f) Motivate the finite result for the following divergent product:  $1 \times 2 \times 3 \times \dots = \sqrt{2\pi}$ .

## 16.<sup>L2</sup> Riemann Surface of Gauss Hypergeometric Function, $K(z)/K(1-z)$ , $\operatorname{erf}^{(-1)}$

a) Carry out the analytical continuation by using Kummer relations [1070★], [3★], [23★], [703★], [1080★], [38★], that are relevant to the analytical continuation ( $1-c, b-a, c-a-b$  not integers in all of the following formulas):

$$\begin{aligned} {}_2F_1(a; b, c; z) &= (1-z)^{c-a-b} {}_2F_1(c-a; c-b, c; z) \\ &= (1-z)^{-a} {}_2F_1\left(a; c-b, c; \frac{z}{z-1}\right) \\ &= (1-z)^{-b} {}_2F_1\left(b; c-a, c; \frac{z}{z-1}\right) \\ &= \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)} {}_2F_1(a; b, a+b-c+1; 1-z) \\ &\quad + \frac{\Gamma(c)\Gamma(a+b-c)}{\Gamma(a)\Gamma(b)} (1-z)^{c-a-b} {}_2F_1(c-a; c-b, c-a-b+1; 1-z) \\ &\quad \text{if } |\arg(1-z)| < \pi \\ &= \frac{\Gamma(c)\Gamma(b-a)}{\Gamma(b)\Gamma(c-a)} (-z)^{-a} {}_2F_1\left(a; 1-c+a, 1-b+a; \frac{1}{z}\right) \\ &\quad + \frac{\Gamma(c)\Gamma(a-b)}{\Gamma(a)\Gamma(c-b)} (-z)^{-b} {}_2F_1\left(b; 1-c+b, b-a+1; \frac{1}{z}\right) \\ &\quad \text{if } |\arg(-z)| < \pi \\ &= \frac{\Gamma(c)\Gamma(b-a)}{\Gamma(b)\Gamma(c-a)} (1-z)^{-a} {}_2F_1\left(a; c-b, a-b+1; \frac{1}{1-z}\right) \end{aligned}$$

$$\begin{aligned}
& + \frac{\Gamma(c)\Gamma(a-b)}{\Gamma(a)\Gamma(c-b)} (1-z)^{-b} {}_2F_1\left(b; c-a, b-a+1; \frac{1}{1-z}\right) \\
& \quad \text{if } |\arg(1-z)| < \pi \\
& = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)} z^{-a} {}_2F_1\left(a; a-c+1, a+b-c+1; 1-\frac{1}{z}\right) \\
& + \frac{\Gamma(c)\Gamma(a+b-c)}{\Gamma(a)\Gamma(b)} (1-z)^{c-a-b} {}_2F_1\left(c-a; 1-a, c-a-b+1; 1-\frac{1}{z}\right) \\
& \quad \text{if } |\arg(z)| < \pi.
\end{aligned}$$

b) Construct pictures of the sheets of the Riemann surface of  ${}_2F_1(1/3; 1/2, 1/6; z)$  that are directly connected with the principal sheet. Carry out the analytical continuation by solving the differential equation for  $w(z) = {}_2F_1(a; b, c; z)$ :

$$z(1-z)w''(z) + (c - (a+b+1)z)w'(z) - abw(z) = 0.$$

c) Construct pictures of the sheets of the Riemann surface of  $w(z) = K(z)/K(1-z)$  [1403★] that are neighboring the principal sheet. Carry out the analytical continuation by solving the Schwarz differential equation for  $K(z)/K(1-z)$ . Find symbolic expressions for the neighboring sheets.

d) Construct a picture of some sheets of the Riemann surface of  $w(z) = \operatorname{erf}^{(-1)}(z)$  in the neighborhood of the point  $z = 1$ .

## 17.<sup>L2</sup> Kummer's 24 Solutions of the Gauss Hypergeometric Differential Equation, Appell Differential Equation

a) The Liouville transformation

$$y(z) = \exp\left(-\frac{1}{2} \int^z p(\xi) d\xi\right) u(z)$$

transforms the differential equation

$$y''(z) + p(z)y'(z) + q(z)y(z) = 0$$

into the normal form  $u''(z) + g(z)u(z) = 0$ . (See also Exercise 11 of Chapter 1.)

Use the Liouville transformation to transform the hypergeometric differential equation

$$z(1-z)y''(z) + (c - (a+b+1)z)y'(z) - aby(z) = 0$$

into normal form. Then, apply a change of the independent variable from  $z$  to  $x$  of the form [646★]

$$z(x) = \frac{\alpha + \beta x}{\gamma + \delta x}$$

and transform the resulting differential equation again to normal form  $w''(x) + h(x)w(x) = 0$ .

One particular solution of the hypergeometric differential equation is  $y(z) = {}_2F_1(a, b; c; z)$ .

Determine all  $\alpha(a, b, c)$ ,  $\beta(a, b, c)$ ,  $\gamma(a, b, c)$ , and  $\delta(a, b, c)$  that leave the above  $g(z)$  form invariant (meaning that  $h(x) = z'(x)^2 g(z(x)) \doteq g(x)$  holds) so that the solution of  $w''(x) + h(x)w(x) = 0$  can again be expressed as a hypergeometric function  ${}_2F_1(a', b'; c'; z)$ , where  $a' = a'(a, b, c)$ ,  $b' = b'(a, b, c)$  and  $c' = c'(a, b, c)$ . Finally, transform the resulting solution back to the original function  $y(z)$  to get a new form of the solution of the hypergeometric differential equation (see [1070★], [3★], [272★], [23★], [623★], [703★], [1080★], and [38★]).

b) The bivariate hypergeometric function  $w(z_1, z_2) = F_1(a; b_1, b_2; c; z_1, z_2)$  fulfills the following coupled system of partial differential equations.

$$\begin{aligned}
 &(1 - z_1) z_1 \frac{\partial^2 w(z_1, z_2)}{\partial z_1^2} + (1 - z_1) z_2 \frac{\partial^2 w(z_1, z_2)}{\partial z_1 \partial z_2} + \\
 &\quad (c - (a + b_1 + 1) z_1) \frac{\partial w(z_1, z_2)}{\partial z_1} - b_1 z_2 \frac{\partial w(z_1, z_2)}{\partial z_2} - a b_1 w(z_1, z_2) = 0 \\
 &(1 - z_2) z_2 \frac{\partial^2 w(z_1, z_2)}{\partial z_2^2} + (1 - z_2) z_1 \frac{\partial^2 w(z_1, z_2)}{\partial z_1 \partial z_2} + \\
 &\quad (c - (a + b_2 + 1) z_2) \frac{\partial w(z_1, z_2)}{\partial z_2} - b_2 z_1 \frac{\partial w(z_1, z_2)}{\partial z_1} - a b_2 w(z_1, z_2) = 0
 \end{aligned}$$

For fixed  $z_2$ , derive an ordinary differential equation of  $F_1(a; b_1, b_2; c; z_1, z_2)$  with respect to  $z_1$  [250★], [381★].

### 18.<sup>L2</sup> Roots of Differentiated Polynomials

- a) Visualize the following theorem: Given a polynomial  $f(z)$  of arbitrary degree over the complex (or real) numbers, all roots of the polynomial  $f'(z)$  lie in the convex hull of the roots of  $f(z)$ . (This is the so-called Gauss–Lucas theorem; see [837★], [877★], [876★], [1228★], [197★], [97★], [1087★], [608★], [1193★], [875★], and [933★]; for a sharpening of this theorem, see [362★].) Look in the standard packages for calculating the convex hull.
- b) Take a random polynomial over the real or complex numbers of degree greater than 10 and show graphically its roots and all of the roots of the polynomial differentiated  $m$  times. The picture suggests that the roots lie on some curves. Try to connect the roots in the “right” order by building a (the “obvious”) continuous version (as a function of  $\alpha$ ) of  $d^\alpha x^n / dx^\alpha$  [791★], [905★], [906★], [907★], [1066★], [908★]. Visualize this generalization of differentiation by itself.

### 19.<sup>L2</sup> Coinciding Bessel Zeros, $\pi$ -Formulas

- a) For  $\mu$  and  $\nu$  nonintegers, it is possible that  $J_\nu(x)$  and  $J_\mu(x)$  have two (or more) zeros in common. Find numerically real values  $\nu, \mu, x, z$ , such that  $J_\nu(x) = J_\mu(x) = 0$  and simultaneously  $J_\nu(z) = J_\mu(z) = 0$  [132★], [1054★].
- b) Ramanujan-like series for  $1/\pi$

$$\frac{1}{\pi} = \sum_{k=0}^{\infty} \frac{a + bk}{k!^3} \left(\frac{1}{2}\right)_k \left(\frac{1}{3}\right)_k \left(\frac{2}{3}\right)_k c^k$$

can be generated based on algebraic solutions  $\alpha_n$  ( $\alpha_n$  is expressable in radicals) of the following transcendental equation for integer  $n > 1$ :

$$\frac{{}_2F_1\left(\frac{1}{3}, \frac{2}{3}; 1; 1 - \alpha_n\right)}{{}_2F_1\left(\frac{1}{3}, \frac{2}{3}; 1; \alpha_n\right)} = \sqrt{n}.$$

The parameters  $a, b$ , and  $c$  algebraic numbers dependent on  $n$  and are defined through  $\alpha_n$  by [290★], [139★], [292★], [293★]

$$\begin{aligned}
 a_n &= \frac{8}{9} \sqrt{\frac{n}{3}} \alpha_n (\alpha_n - 1) \frac{{}_2F_1\left(\frac{4}{3}, \frac{5}{3}; 2; \alpha_n\right)}{{}_2F_1\left(\frac{1}{3}, \frac{2}{3}; 1; \alpha_n\right)} + \frac{1}{\pi {}_2F_1\left(\frac{1}{3}, \frac{2}{3}; 1; \alpha_n\right)^2} \\
 b_n &= \frac{2}{3} \sqrt{3n} \sqrt{1 - 4\alpha_n(1 - \alpha_n)} \\
 c_n &= 4\alpha_n(1 - \alpha_n).
 \end{aligned}$$

(The appearance of  $\pi$  in the formula for  $a$  does not make this a circular definition, the resulting series contains only integers, rationals, and algebraic numbers.) Use numerical techniques to calculate explicit forms of such  $\pi$ -series for  $2 \leq n \leq 20$ .

## 20.<sup>L1</sup> Force-Free Magnetic Fields, Bessel Beams, Gauge Transformation

a) Calculate  $x$  in

$$B_z = x e^{-lz} J_0(rx)$$

$$B_\varphi = a e^{-lz} J_1(rx)$$

$$B_r = l e^{-lz} J_1(rx).$$

( $B_z, B_\varphi, B_r$  are the components of the magnetic field in a cylindrical coordinate system) such that  $\vec{\mathbf{B}}$  is a force-free magnetic field. This means that  $\operatorname{div} \vec{\mathbf{B}} = 0$  and  $\operatorname{curl} \vec{\mathbf{B}} = a \vec{\mathbf{B}}$  hold simultaneously [885★], [133★], [1408★], [1376★].

b) Consider an electromagnetic wave in vacuum with the magnetic field components (in a cylindrical coordinate system) [900★], [903★], [1179★], [957★], [851★], [1122★], [1157★], [400★], [1147★], [202★]

$$B_z = 0$$

$$B_\varphi = J_1(k \sin(\alpha) r) \exp(i(k \cos(\alpha) z - \omega t))$$

$$B_r = 0.$$

Calculate the corresponding electric field  $\{E_z, E_\varphi, E_r\}$  of this wave.

c) A vector potential  $\mathbf{A}_0(r, \varphi)$  of a homogeneous magnetic field of strength  $H$  in  $e_z$ -direction can be chosen in cylindrical coordinates as  $A_\varphi(r, \varphi) = H r/2$ ,  $A_r(r, \varphi) = 0$ ,  $A_z(r, \varphi) = 0$ . (Here  $A_\varphi(r, \varphi)$  is the azimuthal part of the vector potential in cylindrical coordinates and  $r$  is the radius. For domains with polygonal symmetry, it is often useful to have vanishing normal components of the vector potential along the polygon edges [313★]. After a gauge transformation  $\mathbf{A}_0(r, \varphi) \rightarrow \mathbf{A}(r, \varphi) = \mathbf{A}_0(r, \varphi) + \mathbf{G}(r, \varphi)$ , this can be achieved. For a square centered at the origin, with edges parallel to the coordinate axes and edge length  $a$ , the gauge transformation is [312★]

$$G_r(r, \varphi) = H \frac{r^3}{a^6} \left( a^2(a^2 - r^2) + (a^4 - 4r^2 a^2 + 2r^4) \exp\left(1 - \frac{2r^2}{a^2}\right) \operatorname{Ei}\left(\frac{2r^2}{a^2} - 1\right) \right) \sin(4\varphi)$$

$$G_\varphi(r, \varphi) = H \left( \frac{r^3}{a^4} \left( a^2 + (a^2 - 2r^2) \exp\left(1 - \frac{2r^2}{a^2}\right) \operatorname{Ei}\left(\frac{2r^2}{a^2} - 1\right) \right) \cos(4\varphi) \right)$$

$$G_z(r, \varphi) = 0.$$

Verify by explicit calculation that the vector potential  $\mathbf{A}(r, \varphi)$  fulfills the stated properties. Visualize the flowlines of this vector potential and its equipotential lines.

## 21.<sup>L2</sup> Riemann Surface of the Bootstrap Equation

Visualize the Riemann surface of the function  $w(z)$  that is implicitly defined by the equation  $z = 2w - e^w + 1$ .

## 22.<sup>L1</sup> Differential Equation of Powers of Airy Functions, Map Airy Distribution, Zeros of Airy Function

a) Find the (linear) differential equation that is obeyed by  $\operatorname{Ai}(z)^n$  for  $1 \leq n \leq 10$ ,  $n$  integer.

b) Starting from the series expansion of  $\operatorname{Ai}(z)$  for large negative  $z$ , derive the first terms of the expansion of the zeros  $z^{(i)}$  of  $\operatorname{Ai}(z)$  ( $\operatorname{Ai}(z^{(i)}) = 0$ ,  $i = 0, 1, 2, \dots$ ) for large  $i$  in terms of descending powers of  $3\pi/8(4i - 1)$ .

c) In [93★], the “map-Airy” distribution  $p(x)$  was introduced.

$$p(x) = 2 e^{-\frac{2x^3}{3}} (x \operatorname{Ai}(x^2) - \operatorname{Ai}'(x^2))$$

It is a probability distribution. Calculate its asymptotics as  $x \rightarrow \pm\infty$ , the corresponding cumulative distribution function, and its first moment. Calculate  $\int_0^\infty x^2 p(x) dx$ .

### 23.<sup>L2</sup> Differential Equation for Dedekind $\eta$ Function, Darboux–Halphen System

a) The Dedekind Eta function  $\eta(z)$  [805★], [49★], [1196★], [152★], [655★] has the Fourier product representation

$$\eta(z) = e^{\frac{i\pi z}{12}} \prod_{k=1}^{\infty} (1 - e^{2ik\pi z}),$$

where  $\operatorname{Im}(z) > 0$ . The function  $\eta(z)$  obeys a fourth-order, nonlinear differential equation [153★]  $p(\eta(z), \eta'(z), \eta''(z), \eta'''(z), \eta''''(z)) = 0$ , where  $p$  is a multivariate polynomial of total degree 4. Find the polynomial  $p$ .

b) Show that the functions

$$w_1(\tau) = \frac{1}{2} \frac{\partial \ln\left(\frac{\lambda'(\tau)}{\lambda(\tau)}\right)}{\partial \tau}, \quad w_2(\tau) = \frac{1}{2} \frac{\partial \ln\left(\frac{\lambda'(\tau)}{\lambda(\tau)-1}\right)}{\partial \tau}, \quad w_3(\tau) = \frac{1}{2} \frac{\partial \ln\left(\frac{\lambda'(\tau)}{\lambda(\tau)(\lambda(\tau)-1)}\right)}{\partial \tau}$$

where  $\lambda(\tau) = q^{(-1)}(e^{i\pi\tau})$  are solutions of the Darboux–Halphen system [597★]:

$$\begin{aligned} w_1'(z) &= w_1(z)(w_2(z) + w_3(z)) + w_2(z)w_3(z) \\ w_2'(z) &= w_2(z)(w_1(z) + w_3(z)) + w_1(z)w_3(z) \\ w_3'(z) &= w_3(z)(w_1(z) + w_2(z)) + w_1(z)w_2(z). \end{aligned}$$

Here  $q^{(-1)}$  is the inverse of the elliptic nome  $q$  (in *Mathematica* `InverseEllipticNomeQ`). How could one calculate  $q^{(-1)}$ ?

### 24.<sup>L1</sup> Ramanujan Identities for $\varphi$ and $\lambda$ Function

a) For many positive integers  $p, q, r$ , the expression

$$\left( \frac{\vartheta_3(0, \exp(-p\pi))}{\vartheta_3(0, \exp(-q\pi))} \right)^r = \left( \frac{\sum_{k=-\infty}^{\infty} \exp(-k^2 p \pi)}{\sum_{k=-\infty}^{\infty} \exp(-k^2 q \pi)} \right)^r$$

is an algebraic number [136★], [289★], [137★]. (Here,  $\vartheta_3(z, q)$  is the function `EllipticTheta[3, z, q]`.) Use *Mathematica*'s high-precision numerics to find some such integers  $p, q, r$  and the corresponding algebraic numbers.

b) For positive integer  $n$  the expression

$$\lambda_n = \frac{1}{3\sqrt{3}} \left( \frac{\eta\left(\left(1+i\sqrt{\frac{n}{3}}\right)/2\right)}{\eta\left(\left(1+i\sqrt{3n}\right)/2\right)} \right)^6$$

is an algebraic number [1090★], [140★]. (Here,  $\eta(\tau)$  is the function `DedekindEta[\tau]`.) Use *Mathematica*'s high-precision numerics to find the algebraic values for  $1 \leq n \leq 10$ . Find all  $n \leq 100$  such that  $\lambda_n$  is the root of a polynomial of degree four or less.

### 25.<sup>L3</sup> Identities for Gamma Function Values, Identities for Dedekind $\eta$ Function

a) Gamma functions fulfill many identities of the form

$$\frac{\prod_{k=1}^n \Gamma(r_k)^{a_k}}{\prod_{k=1}^m \Gamma(s_k)^{c_k}} = \pi^p \alpha.$$

Here, the  $r_k$  and  $s_k$  are rational numbers,  $a_k$ ,  $c_k$ , and  $p$  are small integers, and  $\alpha$  is an algebraic number. Examples of such identities are [272★], [194★]:

$$\frac{\Gamma(\frac{5}{12})^2}{\Gamma(\frac{1}{4})^2 \Gamma(\frac{2}{3})^2} = \frac{1}{2\pi} \sqrt{-9 + 6\sqrt{3}}$$

$$\frac{\Gamma(\frac{2}{3})^2 \Gamma(\frac{8}{15})^2}{\Gamma(\frac{4}{15})^2 \Gamma(\frac{2}{3})^2} = \frac{3^{7/10}}{\sqrt[5]{5}} \sqrt{\frac{2}{5 + \sqrt{5}}} \sqrt{3} (\sqrt{5} - 1) + \frac{\sqrt{2(5 + \sqrt{5})}}{\sqrt{10 - 2\sqrt{5}} + \sqrt{3} + \sqrt{15}}.$$

Using the functional equations obeyed by the Gamma functions ( $n$  being a positive integer)

$$\Gamma\left(\frac{k}{n}\right) \Gamma\left(1 - \frac{k}{n}\right) = \pi \csc\left(\pi \frac{k}{n}\right)$$

$$\Gamma(nz) = n^n z^{-1/2} (2\pi)^{(1-n)/2} \prod_{k=0}^{n-1} \Gamma\left(z + \frac{k}{n}\right)$$

write a program that generates such identities.

b) The Dedekind Eta function (defined for  $\text{Im}(\tau) > 0$ )

$$\eta(\tau) = e^{\frac{i\pi\tau}{12}} \prod_{k=1}^{\infty} (1 - e^{2i\pi k\tau}) = e^{\frac{i\pi\tau}{12}} \sum_{k=-\infty}^{\infty} (-1)^k e^{k(3k-1)i\pi\tau}$$

fulfills many functional equations of the form [729★], [158★], [135★], [138★], [887★], [545★], [1323★], [1399★], [161★], [978★], [162★], [235★]

$$P(\eta(c_1 \tau), \dots, \eta(c_n \tau)) = 0.$$

Here  $P$  is a multivariate polynomial over the integers and the  $c_i$  are positive integers. Examples of such functional identities are:

$$\begin{aligned} \eta(6\tau)^4 \eta(\tau)^9 - 9 \eta(2\tau)^4 \eta(3\tau)^8 \eta(\tau) + 8 \eta(2\tau)^9 \eta(3\tau)^3 \eta(6\tau) &= 0 \\ \eta(8\tau)^4 \eta(2\tau)^{14} + \eta(\tau)^8 \eta(4\tau)^4 \eta(8\tau)^4 \eta(2\tau)^2 - 2 \eta(\tau)^4 \eta(4\tau)^{14} &= 0 \\ \eta(10\tau)^2 \eta(\tau)^5 - 5 \eta(2\tau)^2 \eta(5\tau)^4 \eta(\tau) + 4 \eta(2\tau)^5 \eta(5\tau) \eta(10\tau) &= 0 \\ \eta(4\tau)^2 \eta(12\tau)^2 \eta(\tau)^8 - 4 \eta(3\tau)^2 \eta(4\tau)^8 \eta(\tau)^2 + 3 \eta(2\tau)^8 \eta(6\tau)^4 &= 0 \\ \eta(\tau)^4 \eta(2\tau) \eta(3\tau)^2 \eta(12\tau)^3 \eta(6\tau)^2 + \eta(2\tau)^3 \eta(3\tau)^6 \eta(12\tau)^3 - 2 \eta(\tau)^2 \eta(4\tau) \eta(6\tau)^9 &= 0 \end{aligned}$$

Conjecture at least 25 more relations of this kind.

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