Approximation Methods in Mathematical Physics Using the Add-on Package MathSymbolica

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Overview

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Exact vs. Approximate Solutions

Applications

Asymptotic Series
Approximate Expansion of Integrals
Approximate Expansion of Sums
Boundary-Layer Theory
WKB Analysis
Integro-differential Equation

References

Bender and Orszag, *Advanced Mathematical Methods for Scientists and Engineers*, McGraw-Hill, 1978.
Arfken and Weber, *Mathematical Methods for Physicists*, 6th ed., Elsevier, 2005.
J. J. Sakurai, *Modern Quantum Mechanics*, Chap 2, Addison-Wesley, 1994.
M. Rahman, "*Integral Equations and their Applications*," Chapter 6 Integro-differential equations, WIT Press, 2007.

MathSymbolica: Symbolic Computing (SC) Package

Overview

Mathematica add-on package that facilitates symbolic computation with mathematical expressions
Over 1,100 functions and own programming language
Display and interpretation of various mathematical expressions like derivatives, integrals, sums, vector operators, brakets, etc. using the traditional notation

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Keywords

Notation,
Manipulation and
Evaluation
of Mathematical Expressions

Motivation

To design and implement a symbolic computing system based on *Mathematica* that can manipulate various mathematical expressions using traditional notation and deferred on-demand evaluation

Objective

To replace hand-written calculation with symbolic computation and software-based automation

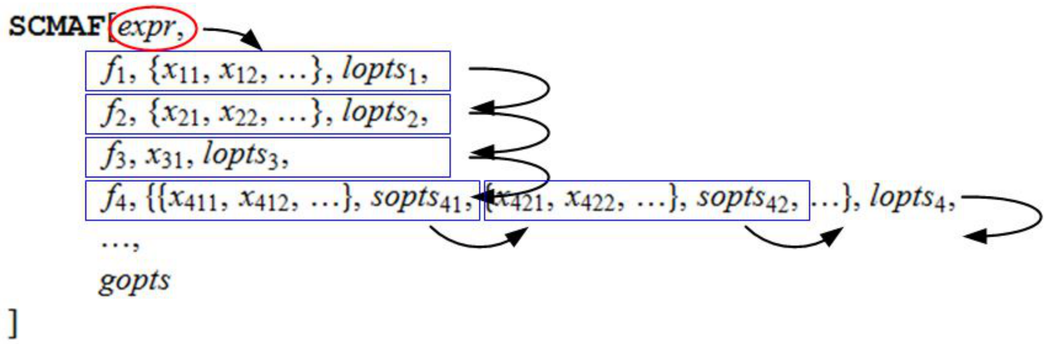
Features

Allows traditional notation for various mathematical expressions
Algebraic manipulation of formulas using symbolic computation

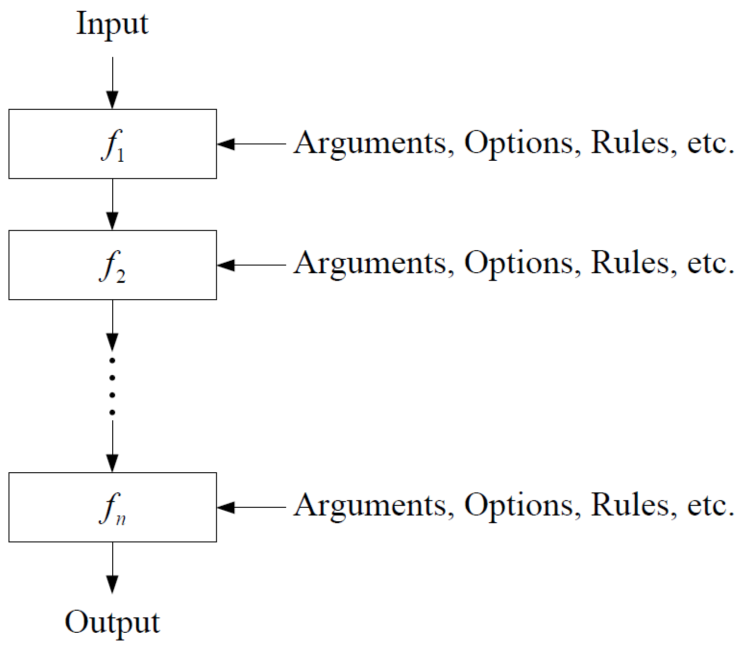
Seamless integration with the computing environment of *Mathematica*
Powerful platform for streamlined manipulation of mathematical expressions

Sequential Execution of Functions

SCMAF function and navigation using the SCMAF Viewer palette



Sequential Execution of Functions



Extended Composition of Functions

Seamless integration with the computing environment of *Mathematica*
Selective targeting of the objects to apply functions

Advantages

Close emulation of hand-written calculation
Allows focusing on concepts and principles rather than tedious, boring, time-consuming and error-prone hand-written calculation
Good readability, enhanced speed and accuracy, and minimization of human errors during calculation
Expressions that closely resemble the traditional mathematical style, e.g., subscripts, derivatives and vector operators

Brief History

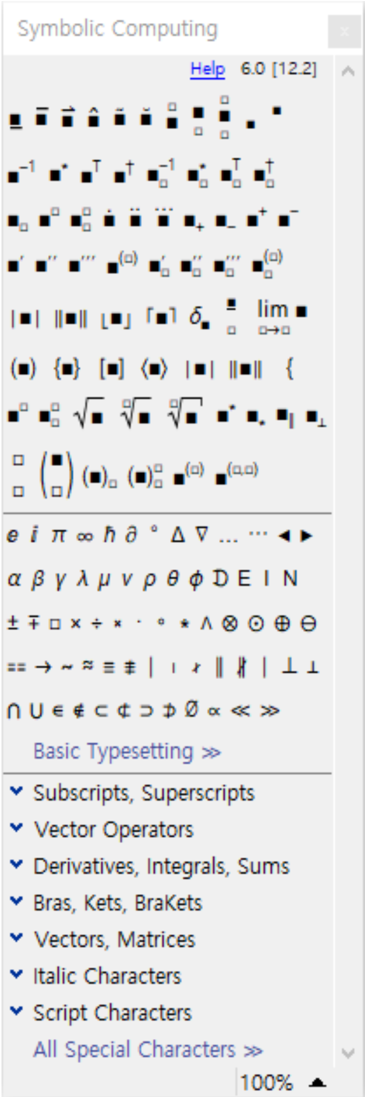
2002. 04: Development started as MiscAlgebra Package (MP)
2007. 11: Presented at the First Korean Mathematica Users Conference
"Advanced Formula Manipulation Using Symbolic Computing"
2011. 08: Renamed to Symbolic Computing (SC) Package
2011. 10: Presented at Wolfram Technology Conference 2011
"Symbolic Computing Package and Its Application to Mathematical Physics"
2012. 02: Version 1.0 beta release after the lecture at Mathematics Dept of Korea University
2012. 04: Version 2.0 beta
2014. 12: Version 3.0 beta
2015. 10: Version 3.1 beta
2016. 06: Version 4.0 beta
2017. 10: Presented at Wolfram Technology Conference 2017
"Mathematics of Series with the Symbolic Computing Package"
2017. 12: Version 4.1 commercial release
2018. 06: Version 5.0 release
2019. 06: Version 5.1 release
2019. 11: Version 5.1.3 release
2021. 01: Version 6.0.0 release
2022. 03: Version 6.1.0 release
2023. 05: The latest release 6.2.0 (May 1, 2023)

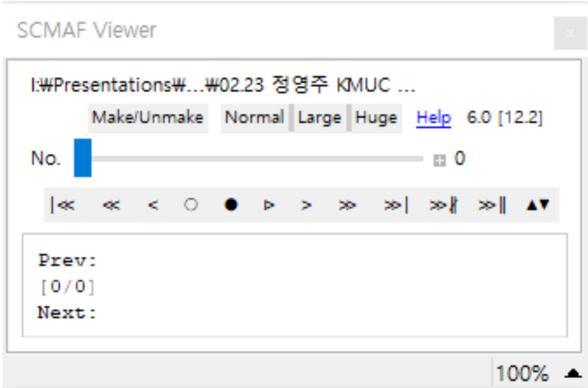
Wolfram Innovator Award 2017

Help for the Symbolic Computing Package

The on-line help for the package is available. It contains documentation of the package functions and examples of the usage of the functions.

The help browser can be opened by clicking Help in the “Symbolic Computing” palette (Palettes menu → Symbolic Computing). The Help link is also available in the “SCMAF Viewer” palette.





New Features in Recent Releases

Number of functions

Version 6.0 (January 24, 2021) : 992
Version 6.1 (March 7, 2022) : 1,033
Version 6.2 (May 1, 2023) : 1,132

Exact vs. Approximate Solutions

Instead of exact solutions, even if they are available, approximate solutions can be much more convenient in applications where they provide sufficient information about the problems at hand.

Examples

1. *Derive the leading behavior of the integral*

$$\int_0^\pi e^{i\,x(t-\sin t)} \cos t\, dt, \quad x \to +\infty.$$

Closed-form evaluation of the integral does not exist.

In[ ]:=
```
SCEvalInt[∫_0^π ⅇ^(ⅈ x (t-Sin[t])) Cos[t] ⅆt]
```

Out[ ]=
```
∫_0^π ⅇ^(ⅈ x (t-Sin[t])) Cos[t] ⅆt
```

2. *Solve the differential equation*

$$\varepsilon\, y'' + (x+1)\, y' - x^2\, y = 0, \quad 0 \le x \le 1, \quad y(0) = 0,\ y(1) = 1, \quad \varepsilon \to 0_+.$$

Closed-form solution does exist, but it is rather complex.

In[ ]:=
```
{ε y'' + (x + 1) y' - x^2 y == 0, y[0] == 0, y[1] == 1}
SCMAF[%, SCDSolve, {All, y[x], x}, Post → SCFuncShort]
```

where $H_n(x)$ is Hermite function and ${}_1F_1\,(a;\, b;\, x)$ is Kummer confluent hypergeometric function (Hypergeometric1F1).

3. *Evaluate the sum*

$$f(x) = \sum_{k=0}^{\infty} (k+x)^{-\alpha}, \quad \alpha > 1,\, x > 0.$$

The sum can be evaluated in closed form.

In[ ]:=
```
f[x] == Σ_(k=0)^∞ (k + x)^-α
SCMAF[%, SCEvalSum, At[2]]
```

Out[ ]=
```
f[x] == Σ_(k=0)^∞ (k + x)^-α
```

Out[ ]=
```
f[x] == HurwitzZeta[α, x]
```

Nevertheless, we wish to express the result using elementary functions.

4. *Solve the integro-differential equation*

$$y''(t) = 1 - t\, e^{-t} - \int_0^t z\, y(z)\, dz, \quad y(0) = y_0,\ y'(0) = y_0'. \quad \left(' \equiv \frac{d}{dt}\right)$$

Direct solution using **`DSolve`** gives a solution that is not so convenient:

In[ ]:=
```
y''[t] == 1 - t e^-t - Integrate[z y[z], {z, 0, t}]
SCMAF[%, SCDSolve, {All, {y[0] == y0, y'[0] == y'0}, y[t], t}, Hold → {y0, y'0}, Post → SCFuncShort]
```

where ${}_pF_q\,(a;\,b;\,z)$ is generalized hypergeometric function (HypergeometricPFQ).

Applications

Asymptotic Series

References

Bender and Orszag, *Advanced Mathematical Methods for Scientists and Engineers*, McGraw-Hill, 1978.

Arfken and Weber, *Mathematical Methods for Physicists*, 6th ed., Elsevier, 2005.

Example 1

(*a*)

Let us consider the Stieltjes series

$$y(x) = \sum_{n=0}^{\infty} (-1)^n \, n! \, x^n.$$

The radius of convergence vanishes.

In[∘]:=
```
R == lim_{n→∞} | a_n / a_{n+1} |
SCMAF[%, RA, {At[2], a_{n_} → (-1)^n n!},
 SCSimpFactorial, At[2], Post → SCEvalLimit]
```

Out[∘]= $R = \lim_{n\to\infty} \left| \frac{a_n}{a_{1+n}} \right|$

$R = \lim_{n\to\infty} \left| \frac{n!}{(1+n)!} \right|$

Out[∘]= $R = 0$

and therefore, the sum diverges for all $x \neq 0$.

The Nth partial sum $s_N(x)$ can be evaluated as

In[∘]:=
```
s_N[x] == Sum[(-1)^n n! x^n, {n, 0, N}]
SCMAF[%, SCEvalSum, At[2],
 FunctionExpand, Γ[0, 1/x], Post → {SCFuncShort, PowerExpand}]
```

Out[∘]= $s_N[x] = \sum_{n=0}^{N} (-1)^n x^n n!$

$s_N[x] = \frac{e^{\frac{1}{x}}}{x} \Gamma\left[0, \frac{1}{x}\right] + \frac{(-1)^N e^{\frac{1}{x}} (1+N)!}{x} \Gamma\left[-1-N, \frac{1}{x}\right]$

Out[∘]= $s_N[x] = -\frac{e^{\frac{1}{x}}}{x} \mathrm{Ei}\left[-\frac{1}{x}\right] + \frac{(-1)^N e^{\frac{1}{x}} (1+N)!}{x} \Gamma\left[-1-N, \frac{1}{x}\right]$

where $\Gamma(a, z)$ is the incomplete gamma function and $-\mathrm{Ei}(-z) = \Gamma(0, z) = E_1(z)$ is the exponential integral function (**`ExpIntegralEi`**). The first term is independent of N and the second term alternates in sign. We put

$$f(x) = -\frac{e^{\frac{1}{x}}}{x}\,\mathrm{Ei}\left(-\frac{1}{x}\right),$$

$$R_N(x) = f(x) - s_N(x) = (-1)^{N+1}\,(N+1)!\,\frac{e^{\frac{1}{x}}}{x}\,\Gamma\left(-N-1,\, \frac{1}{x}\right).$$

This gives

In[ ]:=
```
R_N[x] == ((-1)^(N+1) e^(1/x) (1 + N)!)/x Γ[-1 - N, 1/x]
SCMAF[%, SCMultEq, {All, x^-N},
  Asymptotic, {Γ[-1 - N, 1/x], x → 0}, RA → Arg[x] → 0, Head → Tilde, AddComment → "x → 0₊,"]
```

Out[ ]=
$$R_N[x] == \frac{(-1)^{1+N}\, e^{\frac{1}{x}}\,(1+N)!}{x}\,\Gamma\left[-1-N,\, \frac{1}{x}\right]$$

$$x^{-N} R_N[x] == (-1)^{1+N}\, e^{\frac{1}{x}}\, x^{-1-N}\,(1+N)!\,\Gamma\left[-1-N,\, \frac{1}{x}\right]$$

$$x^{-N} R_N[x] \sim (-1)^{1+N}\, x\,(1+N)!$$

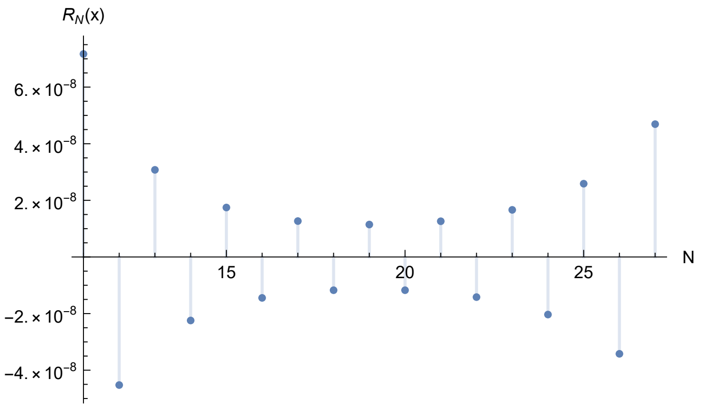
x → 0_+,

which satisfies the conditions for asymptotic series:

$$\lim_{x\to 0} x^{-N} R_N(x) = 0, \quad \text{for fixed } N,$$

$$\lim_{N\to\infty} x^{-N} R_N(x) = \infty, \quad \text{for fixed } x.$$

Plot of $R_N(x)$ vs. N ($x = 0.05$)

Out[ ]=


N	R_N
14	-2.24393×10^{-8}
15	1.74678×10^{-8}
16	-1.44578×10^{-8}
17	1.26790×10^{-8}
18	-1.17442×10^{-8}
19	1.14578×10^{-8}
20	-1.17442×10^{-8}
21	1.26179×10^{-8}
22	-1.41804×10^{-8}
23	1.66376×10^{-8}
24	-2.03440×10^{-8}

From the above plot, $N = 19$ is the optimum value for evaluation of the series when $x = 0.05$. The numerical value of $f(x)$ is

```
f[x] == -(e^(1/x)/x) Ei[-1/x];
SCMAF[%, RA, {All, x → 0.05}, Pre → SCFuncNormal]
```

Out[•]= f[0.05] == 0.954371

(*b*)

The differential equation satisfied by $y(x)$ and the solution:

```
In[•]:= y[x] == Sum[(-1)^n n! x^n, {n, 0, ∞}]
SCMAF[%, SCEqMap,
  List /@ {{All, #&}, {All, D → x}, {All, D → {{x, 2}}}}, PostAll → SCAbbrevFunc,
  Simplify, At[_, 2],
  SCMultEq, {{At[2], x}, {At[3], x^2}}, Post → SCInSum,
  Insert, {All, y' == Sum[(-1)^n n x^(-1+n) n!, {n, 0, ∞}], 2},
  SCSumShiftVar, {At[2], {n, 1}}, Post → {SCFactorSum, SCSumChangeLimits → {{n, 0, ∞}}},
  SCFactorialShift, {(1 + n)!, -1},
  SCTransPoly, {(-1 + n) n, n, n + 1}, Post → {Expand, 2 - 3 × (1 + n)},
  SCExpandSumAll, At[4], Hold → 1 + n,
  SCFactorSum, At[4], ,
  SCEliminate, {All, {Sum[(-1)^n x^n n!, {n, 0, ∞}], Sum[(-1)^n (1 + n)^2 x^n n!, {n, 0, ∞}], Sum[(-1)^n n x^n n!, {n, 0, ∞}]}},
  Post → {SCCollectDerivs → y, SCEqMerge},
  SCDSolve, {All, y, x}, Post → SCFuncShort]
```

Out[•]= $y[x] == \sum_{n=0}^{\infty} (-1)^n x^n n!$

$\{y == \sum_{n=0}^{\infty} (-1)^n x^n n!,\ y' == -\sum_{n=0}^{\infty} (-1)^n (1+n)^2 x^n n!,\ x y' == \sum_{n=0}^{\infty} (-1)^n n x^n n!,$

$x^2 y'' == -\sum_{n=0}^{\infty} (-1)^n x^n n! - 3\sum_{n=0}^{\infty} (-1)^n n x^n n! + \sum_{n=0}^{\infty} (-1)^n (1+n)^2 x^n n!\}$

$y + (1 + 3x) y' + x^2 y'' == 0$

Out[•]= $y == \frac{e^{\frac{1}{x}} c_1}{x} - \frac{e^{\frac{1}{x}} c_2}{x} \mathrm{Ei}\left[-\frac{1}{x}\right]$

Since the first term $x^{-1} e^{1/x}$ diverges as $x \to 0_+$, and since

```
In[•]:= SCAFE[Limit[(e^(1/x)/x) Ei[-1/x], x → 0], SCEvalLimit, All, Pre → SCFuncNormal]
```

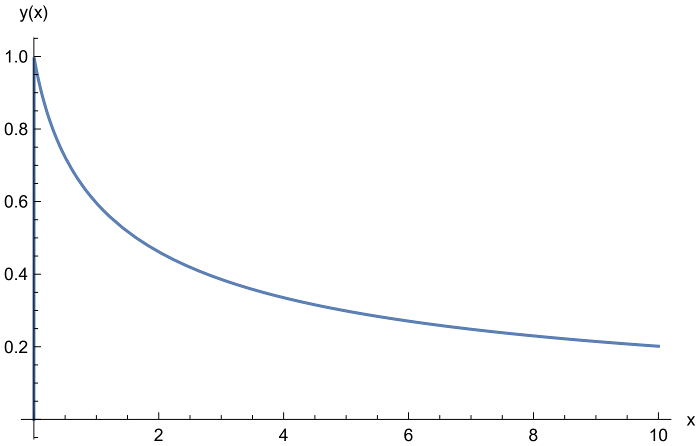
Out[•]= $\lim_{x\to 0} \frac{e^{\frac{1}{x}}}{x} \mathrm{Ei}\left[-\frac{1}{x}\right] == -1$

the constants c_1 and c_2 are determined as $c_1 = 0$, $c_2 = 1$, and therefore, $y(x) = \sum_{n=0}^{\infty} (-1)^n\, n!\, x^n$ is an asymptotic series $(x \to 0_+)$ for

In[ ]:=
```
y == (e^(1/x) c1)/x - (e^(1/x) c2)/x Ei[-1/x] /. {C[1] → 0, C[2] → 1}
```

Out[ ]= $y == -\frac{e^{1/x}}{x}\,\mathrm{Ei}\left[-\frac{1}{x}\right]$

Plot of $-x^{-1}\, e^{1/x}\, \mathrm{Ei}(-1/x)$

Out[ ]=


(*c*)

Using the transformation $x = 1/t$, the differential equation can be put in the form

In[ ]:=
```
y + (1 + 3 x) y′ + x^2 y′′ == 0
SCMAF[%, SCAbbrevDerivPrime, {At[1], x},
  SCTransDeriv, {At[1], TransVar → {x, t, x == 1/t}}, SCCollectDerivs → {y, d^2y/dt^2}]
```

Out[ ]= $y + (1 + 3x)\, y' + x^2 y'' == 0$

$y + (1 + 3x)\frac{dy}{dx} + x^2 \frac{d^2y}{dx^2} == 0$

Out[ ]= $\frac{y}{t^2} - \left(1 + \frac{1}{t}\right)\frac{dy}{dt} + \frac{d^2y}{dt^2} == 0$

It is seen that the differential equation has a regular singularity at $t = 0_+$ ($x = +\infty$). The solution is

In[ ]:=
```
y/t^2 - (1 + 1/t) dy/dt + d^2y/dt^2 == 0
SCMAF[%, SCDSolve, {All, y, t, ReplConst → {-C[2], C[1]}}, Post → SCFuncShort]
```

Out[ ]= $\frac{y}{t^2} - \left(1 + \frac{1}{t}\right)\frac{dy}{dt} + \frac{d^2y}{dt^2} == 0$

Out[ ]= $y == e^t\, t\, c_1 - e^t\, t\, c_2\, \mathrm{Ei}[-t]$

which is identical to the previous result. With $c_1 = 0$, $c_2 = 1$, the power series solution is

In[∘]:=
```
y == e^t t c1 - e^t t c2 Ei[-t]
SCMAF[%, RA, {At[2], {C[1] == 0, C[2] == 1}},
 SCPowerSeries, {At[2], n, Assumptions → t > 0}, Post → PowerExpand, RA → EulerGamma → γ]
```

Out[∘]= $y = e^t\, t\, c_1 - e^t\, t\, c_2\, \text{Ei}[-t]$

$y = -e^t\, t\, \text{Ei}[-t]$

Out[∘]= $y = -t \left(\sum_{n=0}^{\infty} \frac{t^n}{n!}\right) \left(\gamma + \text{Log}[t] + \sum_{n=1}^{\infty} \frac{(-1)^n t^n}{n\, n!}\right)$

where γ is Euler-Mascheroni constant ($\gamma \doteq 0.577216$). Expanding the RHS and combining the sums gives

In[∘]:=
```
y == -t (Sum[t^n/n!, {n, 0, ∞}]) (γ + Log[t] + Sum[(-1)^n t^n/(n n!), {n, 1, ∞}])
SCMAF[%, Expand, At[2],
 SCCombSums, {At[2], ReplVar → k}, SCFactorSum → t^-1,
 SCSumConvertMult, {At[2], n}, SCSepSums → Exponent → False,
 SCEvalSum, Sum[(-1)^k/(k k! (-k + n)!), {k, 1, n}],
 SCSumChangeLimits, {At[2], {n, 0, ∞}}, RA → EulerGamma → γ, Post → SCFuncShort,
 SCExpandSumAll, At[2], Post → {Expand, SCFactorSum → Exponent → False}]
```

Out[∘]= $y = -t \left(\sum_{n=0}^{\infty} \frac{t^n}{n!}\right) \left(\gamma + \text{Log}[t] + \sum_{n=1}^{\infty} \frac{(-1)^n t^n}{n\, n!}\right)$

$y = -\gamma \sum_{n=0}^{\infty} \frac{t^{1+n}}{n!} - \text{Log}[t] \sum_{n=0}^{\infty} \frac{t^{1+n}}{n!} - \sum_{n=0}^{\infty} \frac{t^{1+n}\,(-\gamma - \psi[1+n])}{n!}$

Out[∘]= $y = -\text{Log}[t] \sum_{n=0}^{\infty} \frac{t^{1+n}}{n!} + \sum_{n=0}^{\infty} \frac{t^{1+n}\,\psi[1+n]}{n!}$

where $\psi(z)$ is digamma function given by $\psi(z) = \Gamma'(z)/\Gamma(z)$. This can be written as a power series of x^{-1}:

In[∘]:=
```
y == -Log[t] Sum[t^(1+n)/n!, {n, 0, ∞}] + Sum[t^(1+n) ψ[1+n]/n!, {n, 0, ∞}]
SCMAF[%, RA, {At[2], t → 1/x}, Post → PowerExpand]
```

Out[∘]= $y = -\text{Log}[t] \sum_{n=0}^{\infty} \frac{t^{1+n}}{n!} + \sum_{n=0}^{\infty} \frac{t^{1+n}\,\psi[1+n]}{n!}$

Out[∘]= $y = \text{Log}[x] \sum_{n=0}^{\infty} \frac{x^{-1-n}}{n!} + \sum_{n=0}^{\infty} \frac{x^{-1-n}\,\psi[1+n]}{n!}$

which satisfies the boundary conditions $\lim_{x\to 0_+} y(x) = 1$ and $\lim_{x\to +\infty} y(x) = 0$.

(d)

We now try to convert the sum $\sum_{n=0}^{\infty} (-1)^n\, n!\, x^n$ into an integral form using the identity

$n! = \int_0^\infty e^{-t}\, t^n \, dt \; (n > -1).$

In[ ]:=
```
y[x] == Sum[(-1)^n n! x^n, {n, 0, ∞}]
SCMAF[%, RA, {At[2], n! → Integrate[e^-t t^n, {t, 0, ∞}]},
  SCSumInInt, At[2], Post → {SCPowerMerge, {(-1)^n t^n x^n, n}, SCFactorSum},
  SCEvalSum, At[2]]
```

Out[ ]= $y[x] == \sum_{n=0}^{\infty} (-1)^n x^n n!$

$y[x] == \int_0^\infty e^{-t} \sum_{n=0}^{\infty} (-t\,x)^n \, dt$

Out[ ]= $y[x] == \int_0^\infty \frac{e^{-t}}{1 + t\,x} \, dt$

even though the sum diverges for those values of t such that $|x\,t| \geq 1$. This is called a Stieltjes integral. It can be shown that this integral solution satisfies the same differential equation derived above.

In[ ]:=
```
SCARA[y + (1 + 3 x) y′ + x^2 y″, y == Integrate[e^-t/(1 + t x), {t, 0, ∞}],
  SCEvalDeriv, {At[2], Prime → x},
  SCMergeInts, {At[2], Post → SCDerivSimp → {Variables → t, Derivative → Total}},
  SCEvalIntDeriv, At[2], RA → (e^-t t/(1 + t x)^2)|t==∞ → 0, AddComment → "x > 0."]
```

$y + (1 + 3\,x)\, y' + x^2\, y'' == \int_0^\infty \frac{e^{-t}}{1 + t\,x} \, dt + (1 + 3\,x) \left(\int_0^\infty \frac{e^{-t}}{1 + t\,x} \, dt\right)' + x^2 \left(\int_0^\infty \frac{e^{-t}}{1 + t\,x} \, dt\right)''$

$y + (1 + 3\,x)\, y' + x^2\, y'' == \int_0^\infty \frac{d}{dt} \frac{e^{-t}\, t}{(1 + t\,x)^2} \, dt$

$y + (1 + 3\,x)\, y' + x^2\, y'' == 0$

x > 0.

Repeated integration by parts of $\int_0^\infty e^{-t} \big/ (1 + t\,x) \, dt$ gives

In[ ]:=
```
y[x] == Integrate[e^-t/(1 + t x), {t, 0, ∞}]
SCMAF[%, SCIntByParts, {At[2], e^-t, 6}, Post → SCFactorInt,
  SCFactorInteger, {_Integer, ℤ}, Hold → _Power, FactorOp → False]
```

Out[ ]= $y[x] == \int_0^\infty \frac{e^{-t}}{1 + t\,x} \, dt$

$y[x] == 1 - x + 2\,x^2 - 6\,x^3 + 24\,x^4 - 120\,x^5 + 720\,x^6 \int_0^\infty \frac{e^{-t}}{(1 + t\,x)^7} \, dt$

Out[ ]= $y[x] == 1 - x + 2\,x^2 + (-1) \cdot 2 \cdot 3\,x^3 + 2 \cdot 3 \cdot 4\,x^4 + (-1) \cdot 2 \cdot 3 \cdot 4 \cdot 5\,x^5 + 2 \cdot 3 \cdot 4 \cdot 5 \cdot 6\,x^6 \int_0^\infty \frac{e^{-t}}{(1 + t\,x)^7} \, dt$

hence, we can put

$$y(x) = \sum_{n=0}^{N} (-1)^n \, n! \, x^n + R_N(x),$$

$$R_N(x) = (-1)^{N+1} \, (N+1)! \, x^{N+1} \int_0^\infty \frac{e^{-t}}{(1+t\,x)^{N+2}} \, dt.$$

Using the inequality

In[∘]:=
```
∫_0^∞ e^-t/(1 + t x)^(N+2) dt ≤ ∫_0^∞ e^-t dt
SCMAF[%, SCEvalInt, At[2], AddComment → "x > 0,"]
```

Out[∘]=

$$\int_0^\infty e^{-t} \, (1+t\,x)^{-2-N} \, dt \le \int_0^\infty e^{-t} \, dt$$

$$\int_0^\infty e^{-t} \, (1+t\,x)^{-2-N} \, dt \le 1$$

x > 0,

and hence

$$|R_N(x)| \le (N+1)! \, x^{N+1} \ll x^N, \quad x \to 0_+,$$

it is seen that the Stieltjes series $\sum_{n=0}^{\infty} (-1)^n \, n! \, x^n$ is asymptotic to the Stieltjes integral solution $\int_0^\infty e^{-t} \big/ (1+t\,x) \, dt$.

Approximate Expansion of Integrals

References

Bender and Orszag, *Advanced Mathematical Methods for Scientists and Engineers*, McGraw-Hill, 1978.

Arfken and Weber, *Mathematical Methods for Physicists*, 6th ed., Elsevier, 2005.

Methods of Stationary Phase and Steepest Descents

Method of stationary phase

$$I(x) = \int_a^b f(t)\, e^{i x \psi(t)}\, dt,$$

where $f(t)$, $\psi(t)$, a, b, x are all real.

Method of steepest descents

$$I(x) = \int_C h(z)\, e^{x \rho(z)}\, dz,$$

where $h(z)$ and $\rho(z)$ are analytic functions of z and C is an integration contour in the complex z-plane.

Example 2

Derive the leading behavior of the integral

$$\int_0^\pi e^{i x(t - \sin t)} \cos t\, dt, \quad x \to +\infty.$$

Closed-form evaluation of the integral does not exist.

In[ ]:=
```
SCEvalInt[∫_0^π e^(i x (t-Sin[t])) Cos[t] dt]
```

Out[ ]= $\int_0^\pi e^{i x (t - \text{Sin}[t])} \text{Cos}[t]\, dt$

Use the method of stationary phase to derive the leading behavior. Putting $t = u + i v$ in the exponential factor,

In[ ]:=
```
SCARA[e^(i x (t-Sin[t])), t → u + i v,
 TrigExpand, Sin[_],
 Post → {At[2], SCFactorExp → {x, Post → SCComplex}}, AddComment → "x → +∞."]
```

$e^{i x (t - \text{Sin}[t])} == e^{i x (u + i v - \text{Sin}[u + i v])}$

$e^{i x (t - \text{Sin}[t])} == e^{x (-v + i (u - \text{Cosh}[v] \text{Sin}[u]) + \text{Cos}[u] \text{Sinh}[v])}$

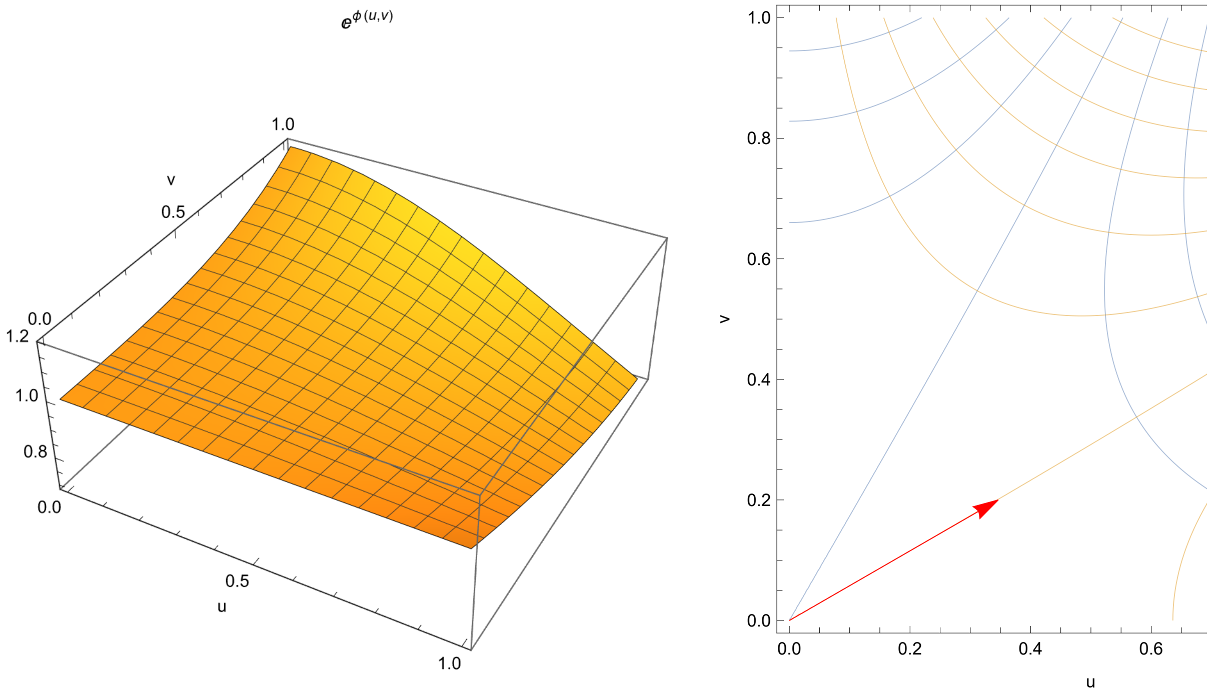
x → +∞.

The real and imaginary parts of the exponent:

$$\phi(u, v) = -v + \sinh v \cos u, \quad \psi(u, v) = u - \cosh v \sin u,$$

Plot of $e^{\phi(u,v)}$ and contour plots of $\phi(u, v)$ and $\psi(u, v)$ in the complex-t plane. The red arrow indicates the path of distorted contour of integration.

Out[∘]=



Taylor expansion of $t - \sin t$ and $\cos t$

In[∘]:=

```
SCAFE[∫_0^π ⅇ^(ⅈ x (t-Sin[t])) Cos[t] ⅆt, SCTaylorSeries, {{t - Sin[t], t, 3}, {Cos[t], t}}, Head → Tilde]
```

Out[∘]= $\int_0^{\pi} e^{i x (t-\mathrm{Sin}[t])} \mathrm{Cos}[t]\, dt \sim \int_0^{\pi} e^{\frac{1}{6} i t^3 x}\, dt$

Variable transformation in the complex-t plane with real s

In[∘]:=

```
SCSolve[ⅈ t^3 x == -s, t]
SCMAF[%, SCComplexToExp, (-1)^p_]
```

Out[∘]= $\left\{\left\{t == -\frac{i\, s^{1/3}}{x^{1/3}}\right\}, \left\{t == \frac{(-1)^{1/6} s^{1/3}}{x^{1/3}}\right\}, \left\{t == \frac{(-1)^{5/6} s^{1/3}}{x^{1/3}}\right\}\right\}$

Out[∘]= $\left\{\left\{t == -\frac{i\, s^{1/3}}{x^{1/3}}\right\}, \left\{t == \frac{e^{\frac{i\pi}{6}} s^{1/3}}{x^{1/3}}\right\}, \left\{t == \frac{e^{\frac{5 i\pi}{6}} s^{1/3}}{x^{1/3}}\right\}\right\}$

There are three possible (deformed) integration contours. Using the second solution which is the closest to the u-axis, we obtain

In[ ]:=
```
SCAFE[∫_0^π e^(1/6 i t^3 x) dt, SCTransInt,
 {All, TransVar → {t, s, t == (e^(iπ/6) s^(1/3))/x^(1/3)}, ReplVar → {s, 0, ∞}}, Post → SCFactorInt,
 SCEvalInt, At[2], Post → {SCComplexToExp, (-1)^(1/6)}]
```

$$\int_0^{\pi} e^{\frac{1}{6} i t^3 x}\, dt == \frac{(-1)^{1/6}}{3 x^{1/3}} \int_0^{\infty} \frac{e^{-s/6}}{s^{2/3}}\, ds$$

Out[ ]= $$\int_0^{\pi} e^{\frac{1}{6} i t^3 x}\, dt == \frac{2^{1/3} e^{\frac{i\pi}{6}} \Gamma\left[\frac{1}{3}\right]}{3^{2/3} x^{1/3}}$$

and hence,

In[ ]:=
```
∫_0^π e^(i x (t-Sin[t])) Cos[t] dt ~ ∫_0^π e^(1/6 i t^3 x) dt
SCMAF[%, RA, {At[2], ∫_0^π e^(1/6 i t^3 x) dt == (2^(1/3) e^(iπ/6) Γ[1/3])/(3^(2/3) x^(1/3))}]
```

Out[ ]= $$\int_0^{\pi} e^{i x (t-\mathrm{Sin}[t])} \mathrm{Cos}[t]\, dt \sim \int_0^{\pi} e^{\frac{1}{6} i t^3 x}\, dt$$

Out[ ]= $$\int_0^{\pi} e^{i x (t-\mathrm{Sin}[t])} \mathrm{Cos}[t]\, dt \sim \frac{2^{1/3} e^{\frac{i\pi}{6}} \Gamma\left[\frac{1}{3}\right]}{3^{2/3} x^{1/3}}$$

Asymptotic Matching

Example 3

Evaluate the integral

$$\int_0^{\pi} e^{i\,x(t-\sin t)} \cos t\, dt, \quad x \to +\infty,$$

including the higher order correction to the stationary phase method.

Use matched asymptotic expansions ($\delta \to 0_+$).

In[ ]:=
```
SCAFE[∫_0^π e^(i x (t-Sin[t])) Cos[t] dt, SCIntChangeInterval, {All, {t, {0, δ}, {δ, π}}},
 RA, {At[2], {∫_0^δ e^(i x (t-Sin[t])) Cos[t] dt → I1, ∫_δ^π e^(i x (t-Sin[t])) Cos[t] dt → I2}}]
```

$$\int_0^{\pi} e^{i x (t-\mathrm{Sin}[t])} \mathrm{Cos}[t]\, dt == \int_0^{\delta} e^{i x (t-\mathrm{Sin}[t])} \mathrm{Cos}[t]\, dt + \int_{\delta}^{\pi} e^{i x (t-\mathrm{Sin}[t])} \mathrm{Cos}[t]\, dt$$

Out[ ]= $$\int_0^{\pi} e^{i x (t-\mathrm{Sin}[t])} \mathrm{Cos}[t]\, dt == I_1 + I_2$$

where

$$I_1 = \int_0^{\delta} e^{i\,x\,(t-\sin t)} \cos t\, dt, \quad I_2 = \int_{\delta}^{\pi} e^{i\,x\,(t-\sin t)} \cos t\, dt, \quad \delta \to 0_+.$$

We approximate I_1 as $x \to +\infty$. The integral can be further approximated.

In[ ]:=
```
I₁ == ∫₀^δ ⅇ^(ⅈ x (t-Sin[t])) Cos[t] ⅆt
SCMAF[%, SCTaylorSeries, {{t - Sin[t], t, 3}, Plus → O[t^5], {Cos[t], t}, Plus → O[t^2]},
  SCTaylorSeries, {At[1], O[_], 2}, Base → _SCIntegrate,
  Post → {SCSimpOrders → {1/x | t, Ordering → False}, Expand, 2 + _, Simplify},
  SCExpandIntAll, At[2], Post → Expand,
  RA, {At[2], ∫₀^δ f_ O[c_. t^a_] ⅆt → O[c δ^(a+1)]}, Post → SCSimpOrders,
  SCIntChangeInterval,
  {At[2], {t, {0, ∞}, {δ, ∞, Multiply → -1}}}, AddComment → "x → ∞, δ → 0₊."]
```

Out[ ]= $I_1 == \int_0^{\delta} e^{i x (t-\sin[t])} \cos[t]\, dt$

$I_1 == \int_0^{\delta} e^{\frac{1}{6} i t^3 x}\, dt + O[\delta^3] + O[x\,\delta^6] + O[x^2\,\delta^{11}]$

$I_1 == \int_0^{\infty} e^{\frac{1}{6} i t^3 x}\, dt - \int_{\delta}^{\infty} e^{\frac{1}{6} i t^3 x}\, dt + O[\delta^3] + O[x\,\delta^6] + O[x^2\,\delta^{11}]$

x → ∞, δ → 0₊.

The first integral has been already obtained using the method of stationary phase:

$$\int_0^{\infty} e^{\frac{1}{6} i t^3 x}\, dt = \frac{2^{1/3}\, e^{\frac{i\pi}{6}}\, \Gamma\left(\frac{1}{3}\right)}{3^{2/3}\, x^{1/3}}.$$

For the second integral, using integration by parts, the expression to be integrated is

In[ ]:=
```
f == D[ⅇ^(1/6 ⅈ t^3 x), t]
SCMAF[%, SCDivide, {At[2], 1/2 ⅈ x}]
```

Out[ ]= $f == \frac{1}{2}\, i\, e^{\frac{1}{6} i t^3 x}\, t^2\, x$

Out[ ]= $f == e^{\frac{1}{6} i t^3 x}\, t^2$

We thus have

In[∘]:=
```
SCAFE[∫_δ^∞ ⅇ^(1/6 ⅈ t^3 x) ⅆt, SCIntByParts, {All, ⅇ^(1/6 ⅈ t^3 x) t^2}, RA → f_{t==∞} → 0, Post → SCFactorInt,
 RA, {At[2], ∫_δ^∞ ⅇ^(1/6 ⅈ t^3 x)/t^3 ⅆt == O[1/(x δ^5)]}, SCSimpOrders → 1/x | δ,
 SCTaylorSeries, {At[2], δ, 0}, Hold → O[_]]
```

$$\int_\delta^\infty e^{\frac{1}{6} i t^3 x}\, dt == \frac{2 i e^{\frac{1}{6} i x \delta^3}}{x \delta^2} - \frac{4 i}{x} \int_\delta^\infty \frac{e^{\frac{1}{6} i t^3 x}}{t^3}\, dt$$

$$\int_\delta^\infty e^{\frac{1}{6} i t^3 x}\, dt == \frac{2 i e^{\frac{1}{6} i x \delta^3}}{x \delta^2} + O\left[\frac{1}{x^2 \delta^5}\right]$$

Out[∘]=
$$\int_\delta^\infty e^{\frac{1}{6} i t^3 x}\, dt == \frac{2 i}{x \delta^2} + O\left[\frac{1}{x^2 \delta^5}\right]$$

where the error integral $\left(\int_\delta^\infty e^{\frac{1}{6} i t^3 x} \big/ t^3\, dt\right)$ is

```
SCAFE[∫_δ^∞ ⅇ^(1/6 ⅈ t^3 x)/t^3 ⅆt, SCIntByParts, {All, ⅇ^(1/6 ⅈ t^3 x) t^2}, RA → f_{t==∞} → 0, Post → SCFactorInt,
 SCChange, {At[2], O[1/(x δ^5)]}]
```

$$\int_\delta^\infty \frac{e^{\frac{1}{6} i t^3 x}}{t^3}\, dt == \frac{2 i e^{\frac{1}{6} i x \delta^3}}{x \delta^5} - \frac{10 i}{x} \int_\delta^\infty \frac{e^{\frac{1}{6} i t^3 x}}{t^6}\, dt$$

Out[∘]=
$$\int_\delta^\infty \frac{e^{\frac{1}{6} i t^3 x}}{t^3}\, dt == O\left[\frac{1}{x \delta^5}\right]$$

The result for I_1 is

In[∘]:=
```
I_1 == ∫_0^∞ ⅇ^(1/6 ⅈ t^3 x) ⅆt - ∫_δ^∞ ⅇ^(1/6 ⅈ t^3 x) ⅆt + O[δ^3] + O[x δ^6] + O[x^2 δ^11]
SCMAF[%, RA, {At[2], {∫_0^∞ ⅇ^(1/6 ⅈ t^3 x) ⅆt == (2^(1/3) ⅇ^(ⅈπ/6) Γ[1/3])/(3^(2/3) x^(1/3)), ∫_δ^∞ ⅇ^(1/6 ⅈ t^3 x) ⅆt == 2ⅈ/(x δ^2) + O[1/(x^2 δ^5)]}},
 Post → SCSimpOrders, AddComment → "x → +∞, δ → 0₊."]
```

Out[∘]=
$$I_1 == \int_0^\infty e^{\frac{1}{6} i t^3 x}\, dt - \int_\delta^\infty e^{\frac{1}{6} i t^3 x}\, dt + O\left[\delta^3\right] + O\left[x \delta^6\right] + O\left[x^2 \delta^{11}\right]$$

$$I_1 == -\frac{2 i}{x \delta^2} + \frac{2^{1/3} e^{\frac{i \pi}{6}} \Gamma\left[\frac{1}{3}\right]}{3^{2/3} x^{1/3}} + O\left[\frac{1}{x^2 \delta^5}\right] + O\left[\delta^3\right] + O\left[x \delta^6\right] + O\left[x^2 \delta^{11}\right]$$

$x \to +\infty,\ \delta \to 0_+$.

To make the error incurred upon integrating by parts smaller than the smallest retained term, we have imposed two new conditions on the magnitude of δ:

In[∘]:=
```
{1/(x δ^2) ≫ δ^3, 1/(x δ^2) ≫ x δ^6, 1/(x δ^2) ≫ 1/(x^2 δ^5)}
SCMAF[%, SCIneqSolve, {At[_], x, Assumptions → {x > 0, δ > 0}}, Delete → {At[1 | 2], 1}]
```

Out[∘]= $\left\{\frac{1}{x\,\delta^2} \gg \delta^3,\ \frac{1}{x\,\delta^2} \gg x\,\delta^6,\ \frac{1}{x\,\delta^2} \gg \frac{1}{x^2\,\delta^5}\right\}$

Out[∘]= $\left\{x \ll \frac{1}{\delta^5},\ x \ll \frac{1}{\delta^4},\ x \gg \frac{1}{\delta^3}\right\}$

and hence, $x^{1/4}\,\delta \to 0_+$ and $x^{1/3}\,\delta \to +\infty$ as $x \to +\infty$.

$$x^{-1/3} \ll \delta \ll x^{-1/4}, \quad x \to +\infty.$$

We thus have

In[∘]:=
```
I1 == -(2 i)/(x δ^2) + (2^(1/3) e^(i π/6) Γ[1/3])/(3^(2/3) x^(1/3)) + O[1/(x^2 δ^5)] + O[δ^3] + O[x δ^6] + O[x^2 δ^11]
SCMAF[%, SCSimpOrders, {At[2], 1/x | δ, Assumptions → x^-1/3 ≪ δ ≪ x^-1/4},
 AddComment → "x → +∞, x^1/4δ → 0+, x^1/3δ → +∞."]
```

Out[∘]= $I_1 = -\frac{2\,i}{x\,\delta^2} + \frac{2^{1/3}\,e^{\frac{i\pi}{6}}\,\Gamma\left[\frac{1}{3}\right]}{3^{2/3}\,x^{1/3}} + O\left[\frac{1}{x^2\,\delta^5}\right] + O\left[\delta^3\right] + O\left[x\,\delta^6\right] + O\left[x^2\,\delta^{11}\right]$

$I_1 = -\frac{2\,i}{x\,\delta^2} + \frac{2^{1/3}\,e^{\frac{i\pi}{6}}\,\Gamma\left[\frac{1}{3}\right]}{3^{2/3}\,x^{1/3}} + O\left[\frac{1}{x^2\,\delta^5}\right] + O\left[x\,\delta^6\right]$

x → +∞, $x^{1/4}\delta$ → 0_+, $x^{1/3}\delta$ → +∞.

For I_2, we integrate by parts three times. The expression to be integrated is

In[∘]:=
```
f == D[e^(i x (t-Sin[t])), t]
SCMAF[%, SCTrigToHalf, 1 - Cos[t], SCDivide → {At[2], 2 i x}]
```

Out[∘]= $f = i\,e^{i\,x\,(t-\mathrm{Sin}[t])}\,x\,(1 - \mathrm{Cos}[t])$

Out[∘]= $f = e^{i\,x\,(t-\mathrm{Sin}[t])}\,\mathrm{Sin}\left[\frac{t}{2}\right]^2$

We thus have

In[1]:=

```
I2 == ∫_δ^π ⅇ^(ⅈ x (t-Sin[t])) Cos[t] ⅆt
SCMAF[%, SCIntByParts, {At[2], ⅇ^(ⅈ x (t-Sin[t])) Sin[t/2]^2},
  Post → {SCFactorExp → ⅈ x, SCFactorInt, Simplify}, Repeat → 3,
  SCTaylorSeries, {(17 Cos[t/2] + 3 Cos[3 t/2]) Csc[t/2]^9, t, -9},
  Expand, At[2], ,
  RA, {At[2], ∫_δ^π ⅇ^(ⅈ x (t-Sin[t]))/t^9 ⅆt == O[1/(x δ^11)]}, SCSimpOrders → 1/x | δ,
  SCTaylorSeries, {{At[2], 1/x, x}, {At[2], δ, 0}}, Hold → O[_]]
```

Out[1]= $I_2 = \int_\delta^\pi e^{i x (t-\mathrm{Sin}[t])} \mathrm{Cos}[t]\, dt$

$$I_2 = \frac{i e^{i \pi x}}{16 x^3} + \frac{i e^{i \pi x}}{2 x} + \frac{i e^{i x (\delta-\mathrm{Sin}[\delta])} \mathrm{Cos}[\delta]}{2 x} \mathrm{Csc}\left[\frac{\delta}{2}\right]^2 - \frac{3 i e^{i x (\delta-\mathrm{Sin}[\delta])}}{16 x^3} \mathrm{Csc}\left[\frac{\delta}{2}\right]^8 - \frac{i e^{i x (\delta-\mathrm{Sin}[\delta])} \mathrm{Cos}[\delta]}{8 x^3} \mathrm{Csc}\left[\frac{\delta}{2}\right]^8 + \frac{640 i}{x^3} \int_\delta^\pi \frac{e^{i x (t-\mathrm{Sin}[t])}}{t^9} dt + \frac{e^{i x (\delta-\mathrm{Sin}[\delta])} \mathrm{Sin}[\delta]}{8 x^2} \mathrm{Csc}\left[\frac{\delta}{2}\right]^6$$

$$I_2 = \frac{i e^{i \pi x}}{16 x^3} + \frac{i e^{i \pi x}}{2 x} + \frac{i e^{i x (\delta-\mathrm{Sin}[\delta])} \mathrm{Cos}[\delta]}{2 x} \mathrm{Csc}\left[\frac{\delta}{2}\right]^2 - \frac{3 i e^{i x (\delta-\mathrm{Sin}[\delta])}}{16 x^3} \mathrm{Csc}\left[\frac{\delta}{2}\right]^8 - \frac{i e^{i x (\delta-\mathrm{Sin}[\delta])} \mathrm{Cos}[\delta]}{8 x^3} \mathrm{Csc}\left[\frac{\delta}{2}\right]^8 + \frac{e^{i x (\delta-\mathrm{Sin}[\delta])} \mathrm{Sin}[\delta]}{8 x^2} \mathrm{Csc}\left[\frac{\delta}{2}\right]^6 + O\left[\frac{1}{x^4 \delta^{11}}\right]$$

Out[2]= $I_2 = -\frac{5 i}{6 x} + \frac{i e^{i \pi x}}{2 x} + \frac{2 i}{x \delta^2} + O\left[\frac{1}{x^4 \delta^{11}}\right]$

where the error integral is

```
SCAFE[∫_δ^π ⅇ^(ⅈ x (t-Sin[t]))/t^9 ⅆt, SCIntByParts, {All, ⅇ^(ⅈ x (t-Sin[t])) Sin[t/2]^2}, Post → SCFactorInt,
  SCChange, {At[2], O[1/(x δ^11)]}]
```

$$\int_\delta^\pi \frac{e^{i x (t-\mathrm{Sin}[t])}}{t^9} dt = -\frac{i e^{i \pi x}}{2 \pi^9 x} + \frac{i e^{i x (\delta-\mathrm{Sin}[\delta])}}{2 x \delta^9} \mathrm{Csc}\left[\frac{\delta}{2}\right]^2 + \frac{i}{2 x} \int_\delta^\pi e^{i t x - i x \mathrm{Sin}[t]} \left(-\frac{9}{t^{10}} \mathrm{Csc}\left[\frac{t}{2}\right]^2 - \frac{1}{t^9} \mathrm{Cot}\left[\frac{t}{2}\right] \mathrm{Csc}\left[\frac{t}{2}\right]^2\right) dt$$

Out[•]= $\int_\delta^\pi \frac{e^{i x (t-\mathrm{Sin}[t])}}{t^9} dt = O\left[\frac{1}{x \delta^{11}}\right]$

The condition on δ is

$$\frac{1}{x} \gg \frac{1}{x^4 \delta^{11}} \quad \longrightarrow \quad x^{-3/11} \ll \delta, \quad x \to +\infty.$$

This is fine, since

$$x^{-1/3} \ll \delta \ll x^{-1/4}, \quad x \to +\infty.$$

The range of δ is

$$x^{-3/11} \ll \delta \ll x^{-1/4} \quad \text{or} \quad x^{-12/44} \ll \delta \ll x^{-11/44}, \quad x \to +\infty.$$

We thus have

In[ ]:=

$$\int_0^\pi e^{i x (t-\text{Sin}[t])} \text{Cos}[t]\, dt == I_1 + I_2$$

```
SCMAF[%, RA,
 {At[2], {I1 == -2 i/(x δ^2) + 2^(1/3) e^(iπ/6) Γ[1/3]/(3^(2/3) x^(1/3)) + O[1/(x^2 δ^5)] + O[x δ^6], I2 == -5 i/(6 x) + i e^(iπx)/(2 x) + 2 i/(x δ^2) + O[1/(x^4 δ^11)]}},
 SCSimpOrders -> {1/x | δ, Assumptions -> x^(-3/11) ≪ δ ≪ x^(-1/4)},
 AddComment -> "x^(-3/11) ≪ δ ≪ x^(-1/4), x -> +∞."]
```

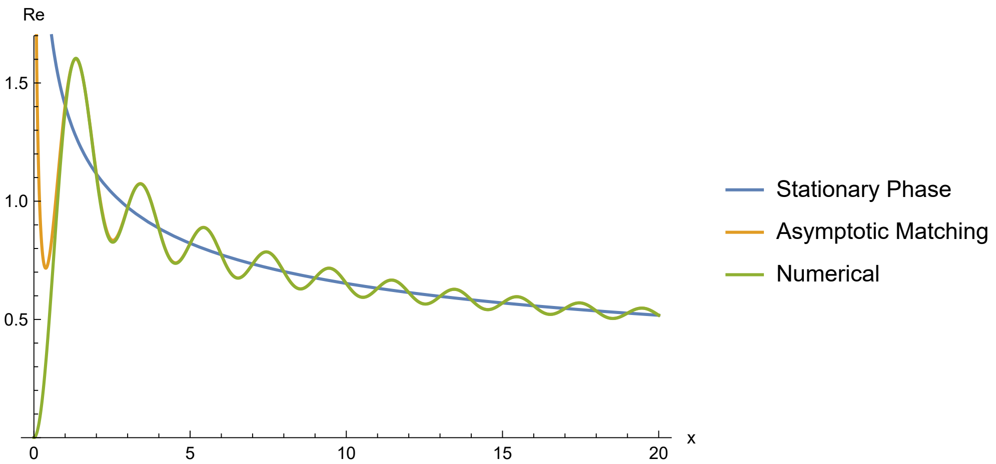
Out[ ]=

$$\int_0^\pi e^{i x (t-\text{Sin}[t])} \text{Cos}[t]\, dt == I_1 + I_2$$

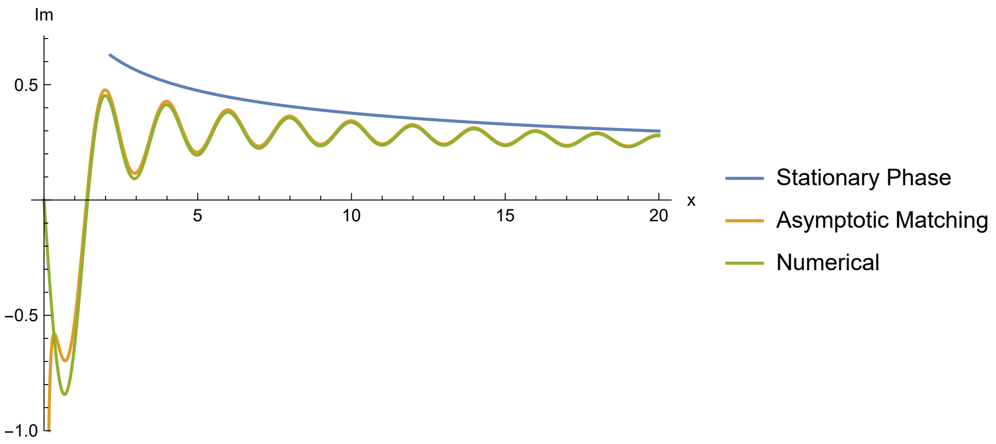
$$\int_0^\pi e^{i x (t-\text{Sin}[t])} \text{Cos}[t]\, dt == -\frac{5 i}{6 x} + \frac{i e^{i \pi x}}{2 x} + \frac{2^{1/3} e^{\frac{i\pi}{6}} \Gamma\left[\frac{1}{3}\right]}{3^{2/3} x^{1/3}} + O\left[x \delta^6\right]$$

$x^{-3/11} \ll \delta \ll x^{-1/4}$, $x \to +\infty$.

Plot of the integrals: stationary phase, asymptotic matching, and numerical



Out[ ]=



Approximate Expansion of Sums

Ref. Bender and Orszag, *Advanced Mathematical Methods for Scientists and Engineers*, McGraw-Hill, 1978.

Euler-Maclaurin Sum Formula

The Euler-Maclaurin series gives the asymptotic expansion of sums of the form

$$F(n) = \sum_{k=0}^{n} f(k), \quad n \to \infty.$$

In terms of the Bernoulli numbers B_n and Bernoulli polynomials $B_n(x)$, the full asymptotic expansion of $F(n)$ is

$$F(n) \sim \frac{1}{2} f(0) + \frac{1}{2} f(n) + \int_0^n f(t)\, dt + \sum_{j=1}^{\infty} \frac{(-1)^j B_{j+1}}{(j+1)!} f^{(j)}(0) -$$

$$\sum_{j=1}^{\infty} \frac{(-1)^j B_{j+1}}{(j+1)!} f^{(j)}(n) + \lim_{m\to\infty} \frac{(-1)^m}{(m+1)!} \sum_{j=0}^{\infty} \int_0^1 B_{m+1}(t)\, f^{(m+1)}(t+j)\, dt.$$

This formula can also evaluate sums like $\sum_{k=0}^{\infty} 1 \big/ \left(k^2 + x^2\right)$, $\sum_{k=0}^{\infty} (k+x)^{-\alpha}$ as $x \to +\infty$.

Example 4

Evaluate the sum

$$f(x) = \sum_{k=0}^{\infty} (k+x)^{-\alpha}, \quad \alpha > 1,\, x > 0.$$

The sum can be evaluated in closed form.

In[∘]:=
```
f[x] == Sum[(k + x)^-α, {k, 0, ∞}]
SCMAF[%, SCEvalSum, At[2]]
```

Out[∘]= $f[x] == \sum_{k=0}^{\infty} (k + x)^{-\alpha}$

Out[∘]= f[x] == HurwitzZeta[α, x]

The Euler-Maclaurin sum formula gives

In[ ]:=
```
SCAFE[∑_{k=0}^{∞} (k + x)^-α, SCEulerMaclaurinSeries,
 {All, Assumptions → {x > 0, α > 1}, Post → SCFuncShort, ReplVar → {t, j, m}},
 RA → {(k + x)^-α_{k==∞} → 0, (k + x)^{-j-α}_{k==∞} → 0},
 SCEvalSum, {∑_{j=1}^{∞} ((-1)^j x^{-j-α} (-α)^(j) B_{1+j})/((1 + j)!), Plus}, AddComment → "α > 1, x → +∞."]
```

$$\sum_{k=0}^{\infty}(k+x)^{-\alpha} ==$$

$$\frac{x^{-\alpha}}{2}+\frac{x^{1-\alpha}}{-1+\alpha}+\lim_{m\to\infty}\frac{(-1)^m}{(1+m)!}\sum_{j=0}^{\infty}\int_0^1(j+t+x)^{-1-m-\alpha}(-\alpha)^{(1+m)}B_{1+m}[t]\,dt+\sum_{j=1}^{\infty}\frac{(-1)^j x^{-j-\alpha}(-\alpha)^{(j)}B_{1+j}}{(1+j)!}$$

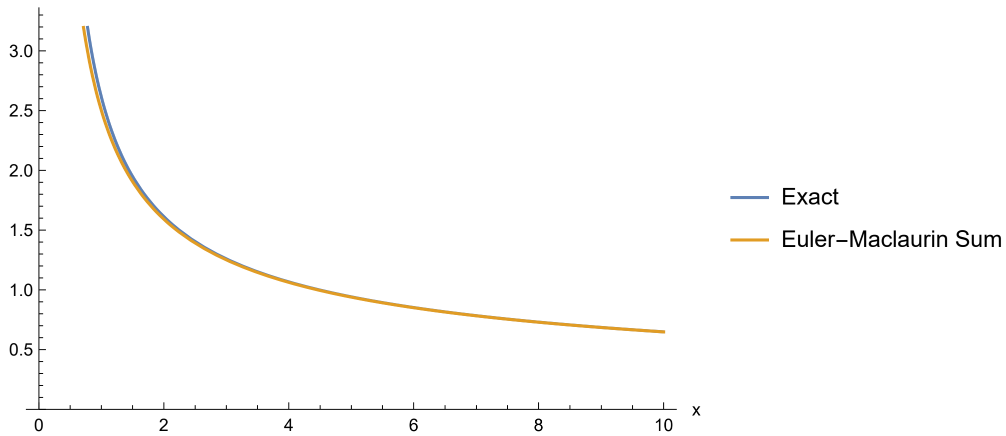
$$\sum_{k=0}^{\infty}(k+x)^{-\alpha} == \frac{x^{-\alpha}}{2}+\frac{x^{1-\alpha}}{-1+\alpha}+\lim_{m\to\infty}\frac{(-1)^m}{(1+m)!}\sum_{j=0}^{\infty}\int_0^1(j+t+x)^{-1-m-\alpha}(-\alpha)^{(1+m)}B_{1+m}[t]\,dt+$$
$$\left(\frac{1}{2}x^{-1-\alpha}\alpha B_2+\frac{1}{6}x^{-2-\alpha}(-\alpha)^{(2)}B_3+-\frac{1}{24}x^{-3-\alpha}(-\alpha)^{(3)}B_4+\cdots\right)$$

α > 1, x → +∞.

For asymptotic expansion ($x \to +\infty$), we ignore the limit and the sum in the RHS, and hence,

$$\sum_{k=0}^{\infty}(k+x)^{-\alpha} \sim \frac{x^{-\alpha}}{2}+\frac{x^{1-\alpha}}{\alpha-1}, \quad \alpha>1,\, x\to+\infty.$$

Plot of the exact sum and the first two terms of Euler-Maclaurin sum ($\alpha = 3/2$)

Out[ ]=


Padé Approximants

The Padé approximant $P_M^N(x)$ is a rational function of the form

$$P_M^N(x) = \frac{\sum_{n=0}^{N} A_n\, x^n}{\sum_{n=0}^{M} B_n\, x^n}, \quad B_0 = 1.$$

For the two-point Padé approximants, J and K are non-negative integers which denote the number of terms to match the Taylor expansion about $x = x_1$ and $x = x_2$, respectively. For the series expansion about 0 and ∞, if the first series has the form $\sum_{n=p}^{\infty} a_n\, x^{n+r}$, we have $J + K = N + M - p - r + 1$. For other cases, $J + K = N + M + 1$. The ranges of J and K are

$0 \le J, K \le J + K.$

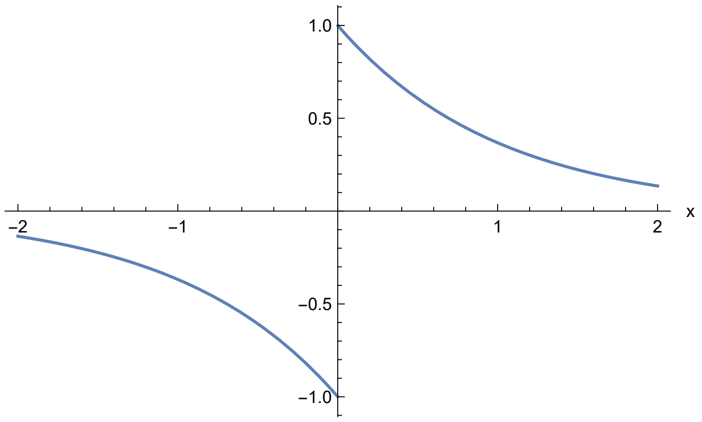
Example 5

Derive the Padé approximants for the piecewise continuous function

$$f(x) = \begin{cases} -e^{x} & x < 0 \\ e^{-x} & x > 0 \end{cases}$$

Plot of $f(x)$

Out[ ]=



Using the two-point Padé approximant with $x_1 = -1$, $x_2 = 1$, we obtain ($N = 3$, $M = 2$, $J = 3$)

In[ ]:=

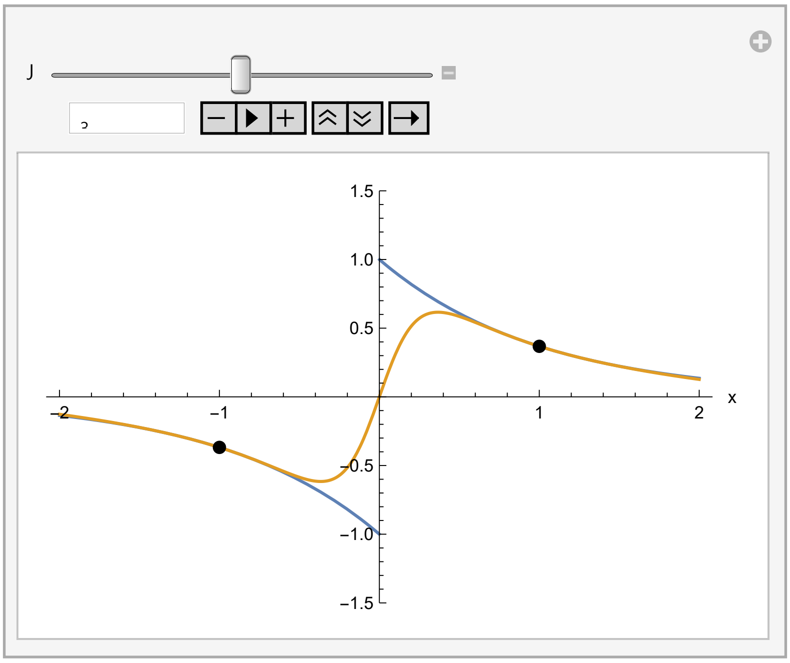
```
f[x] == { -e^x   x < 0
        { e^-x   x > 0
SCMAF[%, SCPadeApproximant, {At[2], 3, 2, 3, {x, -1, 1}}]
```

Out[ ]= $f[x] == \left(\begin{cases} -e^{x} & x < 0 \\ e^{-x} & x > 0 \\ 0 & \text{True} \end{cases} \right)$

Out[ ]= $f[x] == \frac{1}{1 + 7x^2} \left(\frac{9x}{e} - \frac{x^3}{e} \right)$

Plot of $f(x)$ and the Padé approximant with J as a parameter ($N = 3$, $M = 2$)

Out[∘]=



Example 6

Derive the Padé approximants for the divergent Stieltjes series

$$y(x) = \sum_{n=0}^{\infty} (-1)^n x^n n!.$$

The Padé approximant $P_4^4(x)$

In[∘]:=

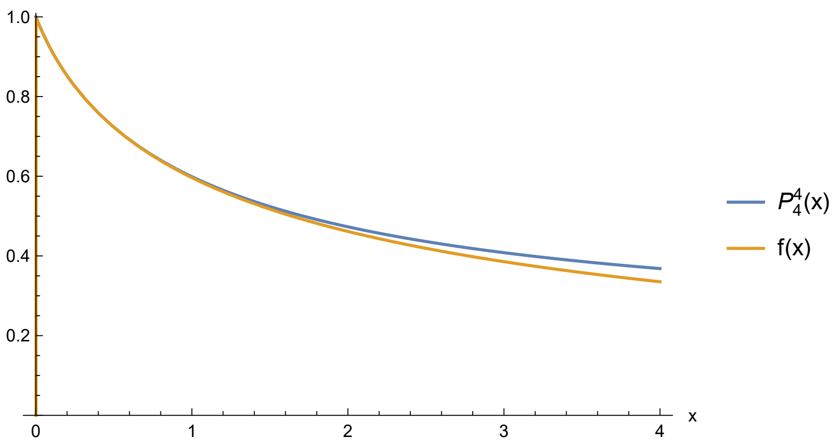
```
y[x] == Sum[(-1)^n x^n n!, {n, 0, ∞}]
SCMAF[%, SCPadeApproximant, {At[2], 4, 4}, RA → {At[1], y[x] → P44[x]}]
```

Out[∘]= $y[x] == \sum_{n=0}^{\infty} (-1)^n x^n n!$

Out[∘]= $P_4^4[x] == \frac{1 + 19 x + 102 x^2 + 154 x^3 + 24 x^4}{1 + 20 x + 120 x^2 + 240 x^3 + 120 x^4}$

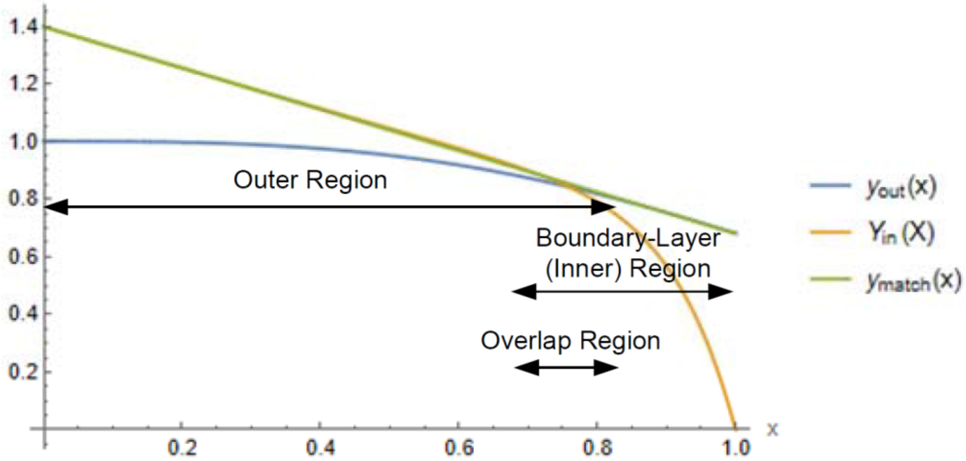
Plot of the Padé approximant $P_4^4(x)$ and $f(x) = -x^{-1} e^{1/x} \text{Ei}(-1/x)$

Out[∘]=



Boundary-Layer Theory

Inner, outer, and overlap regions of the boundary-layer theory



Ref. Bender and Orszag, *Advanced Mathematical Methods for Scientists and Engineers*, McGraw-Hill, 1978.

Second-order Linear Boundary-value Problem

Example 7

Solve the differential equation

$$\varepsilon\, y'' + (x+1)\, y' - x^2\, y = 0, \quad 0 \le x \le 1, \quad y(0) = 0,\ y(1) = 1, \quad \varepsilon \to 0_+.$$

Closed-form solution does exist, but it is rather complex.

In[∘]:=
```
{ε y'' + (x + 1) y' - x^2 y == 0, y[0] == 0, y[1] == 1}
SCMAF[%, SCDSolve, {All, y[x], x}, Post → SCFuncShort]
```

where $H_n(x)$ is Hermite function and ${}_1F_1\,(a, b, x)$ is Kummer confluent hypergeometric function.

For the outer solution, we use $y(x) = \sum_{n=0}^{\infty} \varepsilon^n\, y_n(x)$. Substitution in the differential equation gives

In[ ]:=
```
ε y'' + (x + 1) y' - x^2 y == 0
SCMAF[%, RA, {At[1], y[x] ~ Sum[ε^n y_n[x], {n, 0, ∞}]},
 Post → {SCAbbrevFunc, SCInSum, SCEvalDeriv → Prime → x},
 SCSumShiftVar, {Sum[ε^(1+n) f_, {n, 0, ∞}], {n, -1}},
 SCSumChangeLimits, {At[1], {n, 1, ∞}},
 SCMergeSums, {At[1], Post → SCFactor → ε^n }]
```

Out[ ]= $-x^2\, y + (1+x)\, y' + \varepsilon\, y'' == 0$

$$-\sum_{n=1}^{\infty} x^2\, \varepsilon^n\, y_n + \sum_{n=1}^{\infty} (1+x)\, \varepsilon^n\, y'_n + \sum_{n=1}^{\infty} \varepsilon^n\, y''_{-1+n} - x^2\, y_0 + (1+x)\, y'_0 == 0$$

Out[ ]= $\sum_{n=1}^{\infty} \varepsilon^n \left(-x^2\, y_n + (1+x)\, y'_n + y''_{-1+n}\right) - x^2\, y_0 + (1+x)\, y'_0 == 0$

By equating the coefficients equal to zero, we obtain

$$(x+1)\, y'_0 - x^2\, y_0 = 0, \quad (x+1)\, y'_n - x^2\, y_n = -y''_{n-1}, \quad n \geq 1.$$

The leading-order solution is

In[ ]:=
```
{-x^2 y_0 + (1 + x) y'_0 == 0, y_0[1] == 1}
SCMAF[%, SCDSolve, {All, y_0[x], x, Post → SCSimpExp}, ChangeSign → -1 + x]
```

Out[ ]= $\{-x^2\, y_0 + (1+x)\, y'_0 == 0,\ y_0[1] == 1\}$

Out[ ]= $y_0[x] == \frac{1}{2}\, e^{\frac{1}{2}(1-x)^2}\, (1+x)$

Since $x + 1 > 0$ for $x \geq 0$, there is possibly a boundary layer at $x = 0$. There is no boundary layer at $x = 1$. Suppose there were a boundary layer of thickness δ situated at $x = 0$. Then, we could introduce the inner variables $X = x/\delta$, $Y_{\text{in}}(X) = y(x)$ and rewrite the differential equation as

In[ ]:=
```
ε y'' + (x + 1) y' - x^2 y == 0
SCMAF[%, RA, {At[1], x + 1 → 1},
 SCAbbrevDerivPrime, {At[1], x},
 SCTransDeriv, {All, y == Y_in, TransVar → {x, X, X == x/δ}}]
```

Out[ ]= $-x^2\, y + (1+x)\, y' + \varepsilon\, y'' == 0$

$$-x^2\, y + \frac{dy}{dx} + \varepsilon\, \frac{d^2 y}{dx^2} == 0$$

Out[ ]= $\frac{1}{\delta}\, \frac{dY_{\text{in}}}{dX} + \frac{\varepsilon}{\delta^2}\, \frac{d^2 Y_{\text{in}}}{dX^2} - X^2\, \delta^2\, Y_{\text{in}} == 0$

$$\frac{1}{\delta} \sim \frac{\varepsilon}{\delta^2},\ \delta = \varepsilon;\ \text{OK}.$$

$$\frac{1}{\delta} \sim \delta^2,\ \delta = 1;\ \text{No. Reproduces the outer expansion.}$$

$$\frac{\varepsilon}{\delta^2} \sim \delta^2,\ \delta = \varepsilon^{1/4};\ \text{No. Only the first order term } \frac{d Y_{\text{in}}}{d X} \text{ remains.}$$

The distinguished limit is $\delta = \varepsilon$, in which case we have

In[∘]:=
```
1/δ dY_in/dX + ε/δ^2 d^2Y_in/dX^2 - X^2 δ^2 Y_in == 0
SCMAF[%, RA, {At[1], δ == ε}, SCMultiply → ε,
  RA, {All, Y_in[X] ~ Sum[ε^n Y_n[X], {n, 0, ∞}]}, Post → {SCAbbrevFunc, SCInSum, SCEvalDeriv},
  SCSumShiftVar, {Sum[ε^(3+n) f_, {n, 0, ∞}], {n, -3}},
  SCSumChangeLimits, {At[1], {n, 3, ∞}},
  Post → {Collect → ε, SCMergeSums → Post → SCFactor → ε^n}]
```

Out[∘]= $\frac{1}{\delta}\frac{dY_{in}}{dX} + \frac{\varepsilon}{\delta^2}\frac{d^2 Y_{in}}{dX^2} - X^2 \delta^2 Y_{in} == 0$

$-\sum_{n=3}^{\infty} X^2 \varepsilon^n Y_{-3+n} + \sum_{n=0}^{\infty} \varepsilon^n Y_n' + \sum_{n=0}^{\infty} \varepsilon^n Y_n'' == 0$

Out[∘]= $\sum_{n=3}^{\infty} \varepsilon^n \left(-X^2 Y_{-3+n} + Y_n' + Y_n''\right) + Y_0' + Y_0'' + \varepsilon\,(Y_1' + Y_1'') + \varepsilon^2\,(Y_2' + Y_2'') == 0$

which gives

In[∘]:=
```
{Y'_0 + Y''_0 == 0, Y'_1 + Y''_1 == 0, Y'_2 + Y''_2 == 0, -X^2 Y_(-3+n) + Y'_n + Y''_n == 0}
SCMAF[%, SCMoveTerm, {At[4], X^2 Y_(-3+n)}, AddComment → "n ≥ 3."]
```

Out[∘]= $\{Y_0' + Y_0'' == 0,\ Y_1' + Y_1'' == 0,\ Y_2' + Y_2'' == 0,\ -X^2 Y_{-3+n} + Y_n' + Y_n'' == 0\}$

$\{Y_0' + Y_0'' == 0,\ Y_1' + Y_1'' == 0,\ Y_2' + Y_2'' == 0,\ Y_n' + Y_n'' == X^2 Y_{-3+n}\}$

n ≥ 3.

The leading-order solution subject to the boundary condition $Y_0(0) = 0$ is

In[∘]:=
```
{Y'_0 + Y''_0 == 0, Y_0[0] == 0}
SCMAF[%, SCDSolve, {All, Y_0[X], X, ReplConst → A_0, Post → Collect → {A_0, Expand}}]
```

Out[∘]= $\{Y_0' + Y_0'' == 0,\ Y_0[0] == 0\}$

Out[∘]= $Y_0[X] == \left(1 - e^{-X}\right) A_0$

Asymptotic matching of $y_{\text{out}}(x)$ and $Y_{\text{in}}(X)$ gives the solution for A_0:

In[ ]:=
```
y0[x] == Y0[X]
SCMAF[%, RA, {All, {y0[x] == 1/2 e^(1/2 (1-x)^2) (1 + x), Y0[X] == (1 - e^-X) A0}},
  SCTaylorSeries, {At[1], x, 0}, RA -> {At[2], e^-X -> 0}]
```

Out[ ]= $y_0[x] == Y_0[X]$

$\frac{1}{2} e^{\frac{1}{2}(1-x)^2}(1+x) == (1-e^{-X}) A_0$

Out[ ]= $\frac{\sqrt{e}}{2} == A_0$

The approximation to $y(x)$ in the matching region is

$$y_{\text{match}}(x) = \frac{\sqrt{e}}{2}.$$

The uniform approximation of the solution $y_{\text{unif}}(x)$ is

In[ ]:=
```
yunif[x] == y0[x] + Y0[X] - ymatch[x]
SCMAF[%, RR,
  {At[2], {y0[x] == 1/2 e^(1/2 (1-x)^2) (1 + x), Y0[X] == (1 - e^-X) A0, ymatch[x] == Sqrt[e]/2, A0 == Sqrt[e]/2, X == x/ε}},
  Post -> {Expand, Sqrt[e] _}]
```

Out[ ]= $y_{\text{unif}}[x] == y_0[x] - y_{\text{match}}[x] + Y_0[X]$

Out[ ]= $y_{\text{unif}}[x] == -\frac{1}{2} e^{\frac{1}{2}-\frac{x}{\varepsilon}} + \frac{1}{2} e^{\frac{1}{2}(1-x)^2}(1+x)$

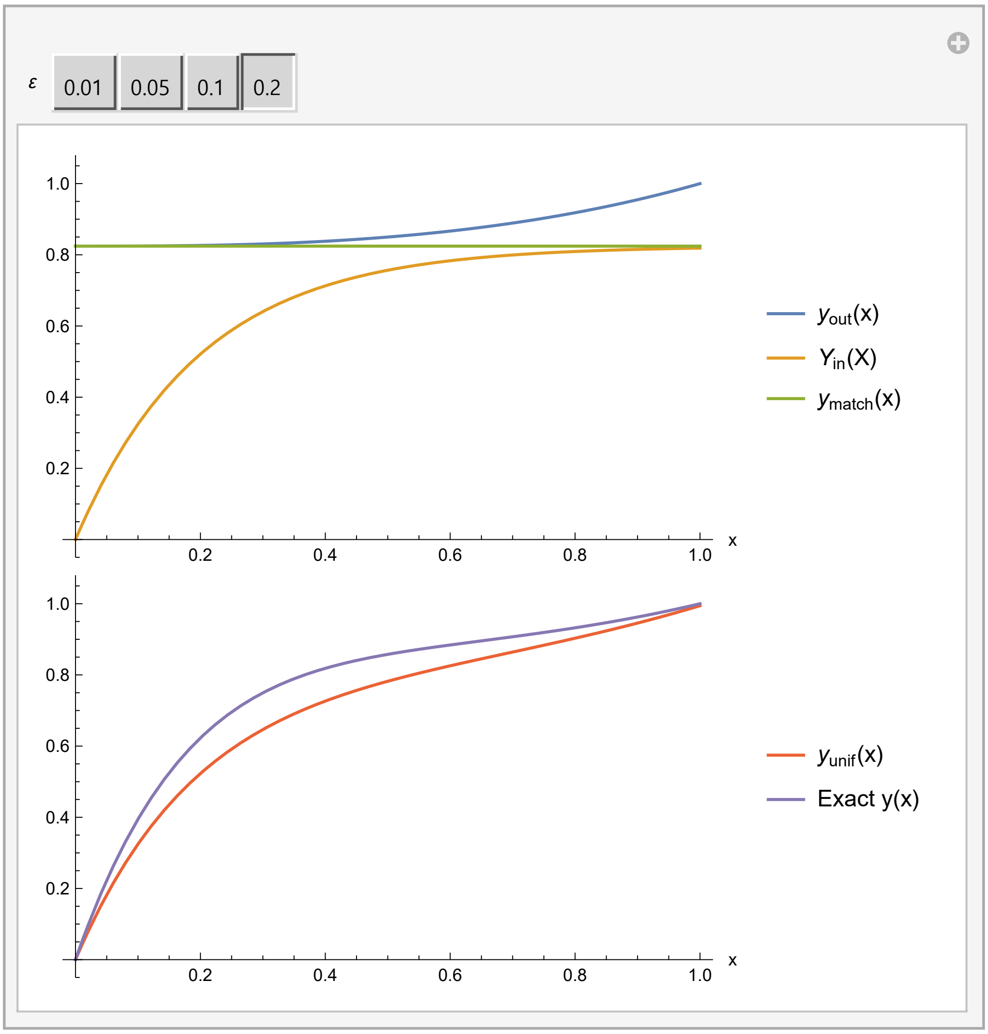
$y_{\text{unif}}(x)$ satisfies the boundary conditions $y(0) = 0$, $y(1) = 1$ within the specified error limit.

In[ ]:=
```
yunif[x] == -1/2 e^(1/2 - x/ε) + 1/2 e^(1/2 (1-x)^2) (1 + x);
SCMAF[%, RA, {All, {{x == 0}, {x == 1}}}]
```

Out[ ]= $\left\{y_{\text{unif}}[0] == 0,\ y_{\text{unif}}[1] == 1 - \frac{1}{2} e^{\frac{1}{2}-\frac{1}{\varepsilon}}\right\}$

Plot of the leading-order $y_{\text{out}}(x)$, $Y_{\text{in}}(X)$, $y_{\text{match}}(x)$, $y_{\text{unif}}(x)$, and the exact solution.

Out[ ]=



Singular Boundary-value Problem

Example 8

Solve the differential equation

$$\varepsilon\, y'' - \frac{1}{x}\, y' - x\, y = 0, \quad 0 \leq x \leq 1, \quad y(0) = 1,\, y(1) = 0, \quad \varepsilon \to 0_+.$$

Since $-1/x$ is negative for $x > 0$, there is no boundary layer at $x = 0$. However, there is a boundary layer at $x = 1$, and the boundary conditions $y(0) = 1$, $y(1) = 0$ uniquely determine the solution.

Substitution of $y(x) = \sum_{n=0}^{\infty} \varepsilon^n\, y_n(x)$ in the differential equation yields

In[∘]:=
```
ε y'' - (1/x) y' - x y == 0
SCMAF[%, RA, {At[1], y[x] ~ Sum[ε^n y_n[x], {n, 0, ∞}]},
  SCEvalDeriv → Prime → x, Post → {SCMultiply → -1, SCAbbrevFunc, SCInSum},
  SCSumShiftVar, {Sum[ε^(1+n) f_, {n, 0, ∞}], {n, -1}},
  SCSumChangeLimits, {At[1], {n, 1, ∞}}, SCMergeSums → Post → SCFactor → ε^n]
```

Out[∘]= $-x\, y - \frac{y'}{x} + \varepsilon\, y'' == 0$

$\sum_{n=0}^{\infty} x\, \varepsilon^n\, y_n + \sum_{n=0}^{\infty} \frac{\varepsilon^n\, y'_n}{x} - \sum_{n=1}^{\infty} \varepsilon^n\, y''_{-1+n} == 0$

Out[∘]= $\sum_{n=1}^{\infty} \varepsilon^n \left(x\, y_n + \frac{y'_n}{x} - y''_{-1+n} \right) + x\, y_0 + \frac{y'_0}{x} == 0$

which gives

$$x\, y_0 + \frac{y'_0}{x} = 0, \quad x\, y_n + \frac{y'_n}{x} = y''_{n-1}, \quad n \geq 1.$$

The solutions are

In[∘]:=
```
{x y_0 + y'_0/x == 0, y_0[0] == 1}
SCMAF[%, SCDSolve, {All, y_0[x], x}]
```

Out[∘]= $\left\{x\, y_0 + \frac{y'_0}{x} == 0,\ y_0[0] == 1\right\}$

Out[∘]= $y_0[x] == e^{-\frac{x^3}{3}}$

In[∘]:=
```
{x y_n + y'_n/x == y''_{n-1}, y_n[0] == 0}
SCMAF[%, RA, {All, n → 1},
  RA, {At[1, 2], y_0[x] == e^(-x^3/3)}, Post → {Simplify, SCEvalDeriv → Prime → x},
  SCDSolve, {All, y_1[x], x}, ChangeSign → -4 + _]
```

Out[∘]= $\left\{x\, y_n + \frac{y'_n}{x} == y''_{-1+n},\ y_n[0] == 0\right\}$

$\left\{x\, y_1 + \frac{y'_1}{x} == e^{-\frac{x^3}{3}}\, x \left(-2 + x^3\right),\ y_1[0] == 0\right\}$

Out[∘]= $y_1[x] == -\frac{1}{6}\, e^{-\frac{x^3}{3}}\, x^3 \left(4 - x^3\right)$

and so on. Up to the first order in ε, the outer solution $y_{\text{out}}(x)$ is

In[ ]:=
```
y_out[x] ~ y_0[x] + ε y_1[x] + O[ε^2]
SCMAF[%, RA, {At[2], {y_0[x] == e^(-x^3/3), y_1[x] == -1/6 e^(-x^3/3) x^3 (4 - x^3)}},
  SCFactor → e^(-x^3/3), Collect → {{e^(-x^3/3), ε}}, AddComment → "ε → 0_+."]
```

Out[ ]= $y_{\text{out}}[x] \sim O[\varepsilon^2] + y_0[x] + \varepsilon\, y_1[x]$

$y_{\text{out}}[x] \sim e^{-\frac{x^3}{3}} \left(1 + \varepsilon \left(-\frac{2\, x^3}{3} + \frac{x^6}{6}\right)\right) + O[\varepsilon^2]$

ε → 0₊.

A boundary layer of thickness ε is required at $x = 1$. If δ is the thickness of the boundary layer, using the variable transformation $X = (1 - x)/\delta$, the differential equation becomes

In[ ]:=
```
ε y'' - 1/x y' - x y == 0
SCMAF[%, SCAbbrevDerivPrime, {At[1], x}, SCMultiply → x,
  SCTransDeriv, {All, y == Y_in, TransVar → {x, X, X == (1 - x)/δ}}, RA → X δ → 0]
```

Out[ ]= $-x\, y - \frac{y'}{x} + \varepsilon\, y'' == 0$

$-x^2\, y - \frac{dy}{dx} + x\, \varepsilon \frac{d^2 y}{dx^2} == 0$

Out[ ]= $\frac{1}{\delta} \frac{dY_{\text{in}}}{dX} + \frac{\varepsilon}{\delta^2} \frac{d^2 Y_{\text{in}}}{dX^2} - Y_{\text{in}} == 0$

The distinguished limit is $\delta = \varepsilon$:

$$\frac{1}{\delta} \sim \frac{\varepsilon}{\delta^2},\ \delta = \varepsilon;\ \text{OK.}$$

$$\frac{1}{\delta} \sim 1,\ \delta = 1;\ \text{No. Reproduces the outer expansion.}$$

$$\frac{\varepsilon}{\delta^2} \sim 1,\ \delta = \varepsilon^{1/2};\ \text{No. Only the first order term } \frac{dY_{\text{in}}}{dX} \text{ remains.}$$

For the inner solution, we put

$$Y_{\text{in}}(X) = \sum_{n=0}^{\infty} \varepsilon^n\, Y_n(X), \quad X = \frac{1 - x}{\varepsilon}, \quad \varepsilon \to 0_+.$$

Substitution in the differential equaiton gives

In[∘]:=
```
ε y'' - (1/x) y' - x y == 0
SCMAF[%, SCAbbrevDerivPrime, {At[1], x},
  SCTransDeriv, {At[1], y == Y_in, TransVar → {x, X, X == (1 - x)/ε}},
  Post → {Expand, SCMultiply → ε (1 - X ε)},
  RA, {All, Y_in[X] ~ Sum[ε^n Y_n[X], {n, 0, ∞}]}, Post → {SCAbbrevFunc, SCInSum, SCEvalDeriv},
  SCSumShiftVar, {Sum[ε^(n+s_) f_, {n, 0, ∞}], {n, -s}},
  SCSumChangeLimits, {At[1], {n, 3, ∞}},
  Post → {Collect → ε, SCMergeSums → Post → SCFactor → ε^n, Expand}]
```

Out[∘]= $-x\,y - \frac{y'}{x} + \varepsilon\, y'' == 0$

$$-\sum_{n=3}^{\infty} X^2 \varepsilon^n Y_{-3+n} + 2\sum_{n=2}^{\infty} X \varepsilon^n Y_{-2+n} - \sum_{n=1}^{\infty} \varepsilon^n Y_{-1+n} + \sum_{n=0}^{\infty} \varepsilon^n Y'_n - \sum_{n=1}^{\infty} X \varepsilon^n Y''_{-1+n} + \sum_{n=0}^{\infty} \varepsilon^n Y''_n == 0$$

Out[∘]= $$\sum_{n=3}^{\infty} \varepsilon^n \left(-X^2 Y_{-3+n} + 2\,X\,Y_{-2+n} - Y_{-1+n} + Y'_n - X\,Y''_{-1+n} + Y''_n\right) + Y'_0 + Y''_0 + \varepsilon\,(-Y_0 + Y'_1 - X\,Y''_0 + Y''_1) + \varepsilon^2\,(2\,X\,Y_0 - Y_1 + Y'_2 - X\,Y''_1 + Y''_2) == 0$$

Equating the coefficients of ε and its powers to zero gives

In[∘]:=
```
{Y'_0 + Y''_0 == 0, -Y_0 + Y'_1 - X Y''_0 + Y''_1 == 0, 2 X Y_0 - Y_1 + Y'_2 - X Y''_1 + Y''_2 == 0,
  -X^2 Y_{-3+n} + 2 X Y_{-2+n} - Y_{-1+n} + Y'_n - X Y''_{-1+n} + Y''_n == 0}
SCMAF[%, SCSepVars, {{At[2], Y_1}, {At[3], Y_2}, {At[4], Y_n}}, AddComment → "n ≥ 3."]
```

Out[∘]= $\{Y'_0 + Y''_0 == 0,\ -Y_0 + Y'_1 - X\,Y''_0 + Y''_1 == 0,\ 2\,X\,Y_0 - Y_1 + Y'_2 - X\,Y''_1 + Y''_2 == 0,\ -X^2 Y_{-3+n} + 2\,X\,Y_{-2+n} - Y_{-1+n} + Y'_n - X\,Y''_{-1+n} + Y''_n == 0\}$

$\{Y'_0 + Y''_0 == 0,\ Y'_1 + Y''_1 == Y_0 + X\,Y''_0,\ Y'_2 + Y''_2 == -2\,X\,Y_0 + Y_1 + X\,Y''_1,\ Y'_n + Y''_n == X^2 Y_{-3+n} - 2\,X\,Y_{-2+n} + Y_{-1+n} + X\,Y''_{-1+n}\}$

n ≥ 3.

The solutions for Y_0 and Y_1 are

In[∘]:=
```
{Y'_0 + Y''_0 == 0, Y_0[0] == 0}
SCMAF[%, SCDSolve, {All, Y_0[X], X, ReplConst → -A_0, Post → Simplify}]
```

Out[∘]= $\{Y'_0 + Y''_0 == 0,\ Y_0[0] == 0\}$

Out[∘]= $Y_0[X] == \left(-1 + e^{-X}\right) A_0$

In[ ]:=
```
{Y′₁ + Y″₁ == Y₀ + X Y″₀, Y₁[0] == 0}
SCMAF[%, RA, {At[1, 2], Y₀[X] == (-1 + e^-X) A₀}, SCEvalDeriv → Prime → X,
  SCDSolve, {All, Y₁[X], X, ReplConst → A₁, Post → Expand},
  Collect, {At[2], {e^-X, X}}, RA → A₁ → A₁ - 2 A₀]
```

Out[ ]= $\{Y_1' + Y_1'' == Y_0 + X Y_0'', Y_1[0] == 0\}$

$$Y_1[X] == 2 A_0 - 2 e^{-X} A_0 - X A_0 - 2 e^{-X} X A_0 - \frac{1}{2} e^{-X} X^2 A_0 + A_1 - e^{-X} A_1$$

Out[ ]= $Y_1[X] == -X A_0 + e^{-X}\left(-2 X A_0 - \frac{X^2 A_0}{2} - A_1\right) + A_1$

The inner solution is

In[ ]:=
```
Y_in[X] ~ Y₀[X] + ε Y₁[X]
SCMAF[%, RA, {At[2], {Y₀[X] == (-1 + e^-X) A₀, Y₁[X] == -X A₀ + e^-X (-2 X A₀ - X² A₀/2 - A₁) + A₁}}]
```

Out[ ]= $Y_{in}[X] \sim Y_0[X] + \varepsilon Y_1[X]$

Out[ ]= $Y_{in}[X] \sim \left(-1 + e^{-X}\right) A_0 + \varepsilon\left(-X A_0 + e^{-X}\left(-2 X A_0 - \frac{X^2 A_0}{2} - A_1\right) + A_1\right)$

Matching the outer expansion, the constants A_0 and A_1 are

In[ ]:=
```
y_out[x] == Y_in[X]
SCMAF[%, RA, {All, {y_out[x] ~ e^(-x³/3) (1 + ε (-2 x³/3 + x⁶/6)),
    Y_in[X] ~ (-1 + e^-X) A₀ + ε (-X A₀ + e^-X (-2 X A₀ - X² A₀/2 - A₁) + A₁)}}, RA → {e^-X → 0, X → (1 - x)/ε},
  SCTaylorSeries, {At[1], {ε, 1 - x}, x}, SCExpandMult → At[2], ,
  SCCollectPoly, {All, {ε, x}, Coefficient → True}, Post → Thread,
  SCSolve, {All, {A₀, A₁}}]
```

Out[ ]= $y_{out}[x] == Y_{in}[X]$

$$\frac{1}{e^{1/3}} + \frac{1-x}{e^{1/3}} - \frac{\varepsilon}{2 e^{1/3}} == -A_0 - (1-x) A_0 + \varepsilon A_1$$

$$\left\{\frac{2}{e^{1/3}} == -2 A_0, -\frac{1}{e^{1/3}} == A_0, -\frac{1}{2 e^{1/3}} == A_1\right\}$$

Out[ ]= $\left\{A_0 == -\frac{1}{e^{1/3}}, A_1 == -\frac{1}{2 e^{1/3}}\right\}$

and we find that the inner solution is

In[•]:=

```
Yin[X] ~ (-1 + e^-X) A0 + ε (-X A0 + e^-X (-2 X A0 - X^2 A0/2 - A1) + A1)
SCMAF[%, RA, {At[2], {A0 == -1/e^(1/3), A1 == -1/(2 e^(1/3))}}, Post → Simplify,
  SCExpandMult, At[2], Post → SCFactor → {e^(-1/3), Post → Collect → {{e^-X, ε, X}}}]
```

Out[•]=
$$Y_{in}[X] \sim \left(-1+e^{-X}\right) A_0 + \varepsilon \left(-X A_0 + e^{-X}\left(-2 X A_0 - \frac{X^2 A_0}{2} - A_1\right) + A_1\right)$$

$$Y_{in}[X] \sim \frac{1}{2} e^{-\frac{1}{3}-X}\left(-2 + \left(1+4X+X^2\right)\varepsilon + e^X\left(2+(-1+2X)\varepsilon\right)\right)$$

Out[•]=
$$Y_{in}[X] \sim \frac{1}{e^{1/3}}\left(1+\left(-\frac{1}{2}+X\right)\varepsilon + e^{-X}\left(-1+\varepsilon\left(\frac{1}{2}+2X+\frac{X^2}{2}\right)\right)\right)$$

In the intermediate limit, $y_{match}(x)$ is

In[•]:=

```
ymatch[x] == 1/e^(1/3) + (1 - x)/e^(1/3) - ε/(2 e^(1/3))
SCMAF[%, Collect, {At[2], ε, Together}]
```

Out[•]=
$$y_{match}[x] == \frac{1}{e^{1/3}} + \frac{1-x}{e^{1/3}} - \frac{\varepsilon}{2 e^{1/3}}$$

Out[•]=
$$y_{match}[x] == \frac{2-x}{e^{1/3}} - \frac{\varepsilon}{2 e^{1/3}}$$

and the uniform approximation to $y(x)$ for $0 \le x \le 1$, accurate to order ε, is

In[•]:=

```
yunif[x] == yout[x] + Yin[X] - ymatch[x]
SCMAF[%, RR, {At[2], {yout[x] ~ e^(-x^3/3) (1 + ε (-2 x^3/3 + x^6/6)),
   Yin[X] ~ 1/e^(1/3) (1 + (-1/2 + X) ε + e^-X (-1 + ε (1/2 + 2 X + X^2/2))), ymatch[x] == (2 - x)/e^(1/3) - ε/(2 e^(1/3))}}]
```

Out[•]=
$$y_{unif}[x] == -y_{match}[x] + y_{out}[x] + Y_{in}[X]$$

Out[•]=
$$y_{unif}[x] == -\frac{2-x}{e^{1/3}} + \frac{\varepsilon}{2e^{1/3}} + e^{-\frac{x^3}{3}}\left(1+\varepsilon\left(-\frac{2x^3}{3}+\frac{x^6}{6}\right)\right) + \frac{1}{e^{1/3}}\left(1+\left(-\frac{1}{2}+X\right)\varepsilon + e^{-X}\left(-1+\varepsilon\left(\frac{1}{2}+2X+\frac{X^2}{2}\right)\right)\right)$$

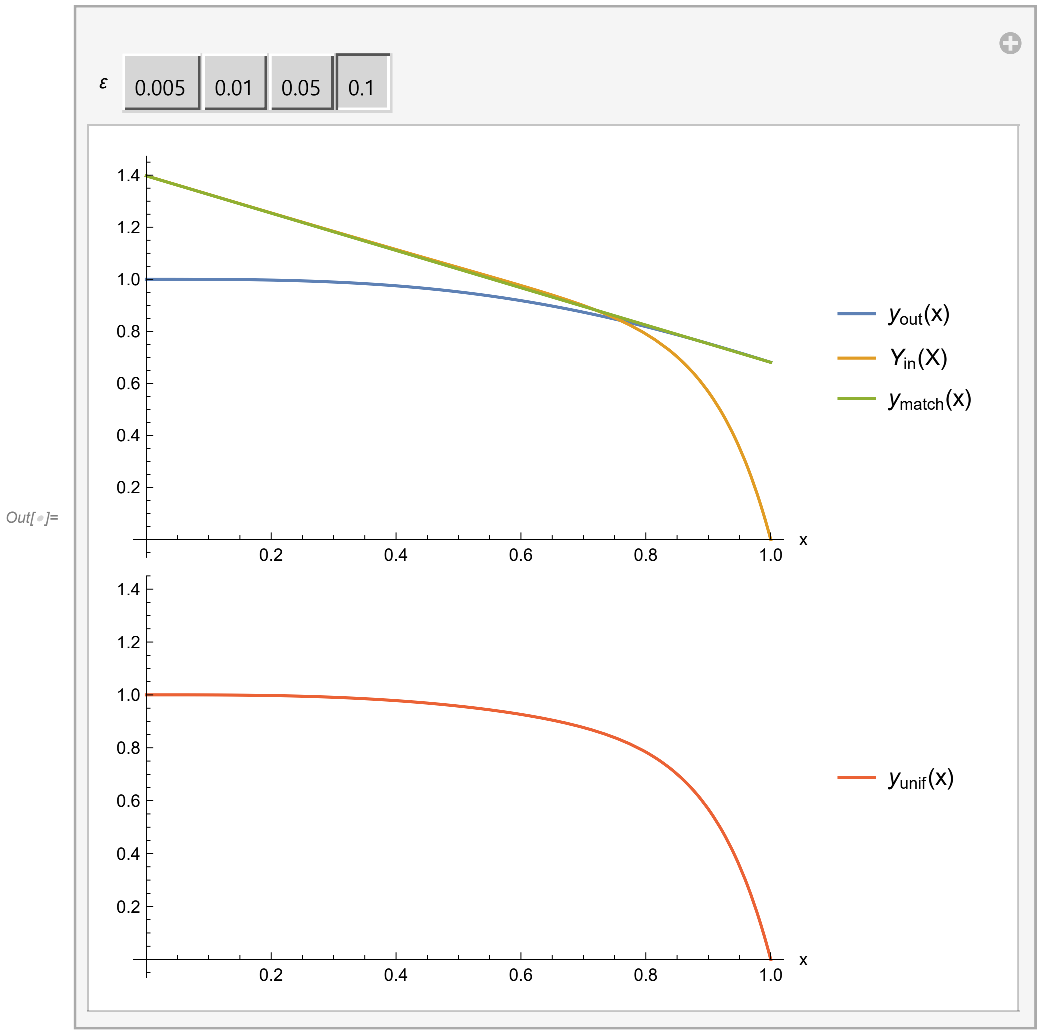
$y_{unif}(x)$ satisfies the boundary conditions $y(0) = 1$, $y(1) = 0$ within the specified error limit.

In[•]:=

```
yunif[x] ==
  -(2 - x)/e^(1/3) + ε/(2 e^(1/3)) + e^(-x^3/3) (1 + ε (-2 x^3/3 + x^6/6)) + 1/e^(1/3) (1 + (-1/2 + X) ε + e^-X (-1 + ε (1/2 + 2 X + X^2/2)));
SCMAF[%, RA, {All, X → (1 - x)/ε}, RA → {{x == 0}, {x == 1}}, Post → Simplify]
```

Out[•]=
$$\left\{y_{unif}[0] == 1 + \frac{e^{-\frac{1}{3}-\frac{1}{\varepsilon}}(1+\varepsilon)^2}{2\varepsilon},\ y_{unif}[1] == 0\right\}$$

Plot of $y_{out}(x)$, $Y_{in}(X)$, $y_{match}(x)$, and $y_{unif}(x)$. The differential equation cannot be solved numerically due to the singularity at $x = 0$.



WKB Analysis

Approximate solution of a differential equation is assumed to be of the form:

$$\psi(x, t) = \sqrt{\rho(x, t)} \exp\left(\frac{i S(x, t)}{\hbar}\right).$$

The WKB method was invented by Lord Rayleigh, but later applied to quantum mechanics problems by G. Wentzel, H. Kramers, and L. Brillouin.

Ref. J. J. Sakurai, *Modern Quantum Mechanics*, Chap 2, Addison-Wesley, 1994.

Airy Functions

Example 9

Solve the differential equation

$$\frac{d^2 y}{d x^2} - x y = 0, \quad y(x) \to 0 \text{ as } x \to +\infty.$$

The exact solution

In[∘]:=
```
d²y/dx² - x y == 0
SCMAF[%, SCDSolve, {All, y[x], x, ReplConst → {A, B}}, Post → SCFuncShort]
```

Out[∘]= $-x\, y + \frac{d^2 y}{d x^2} == 0$

Out[∘]= $y[x] == A\, \mathrm{Ai}[x] + B\, \mathrm{Bi}[x]$

The asymptotic solution in the limit $x \to +\infty$ is

In[∘]:=
```
y[x] == A Ai[x] + B Bi[x]
SCMAF[%, SCAsympSeries, {At[2], Assumptions → x > 0}, Head → Tilde]
```

Out[∘]= $y[x] == A\, \mathrm{Ai}[x] + B\, \mathrm{Bi}[x]$

Out[∘]= $y[x] \sim \frac{A\, e^{-\frac{2 x^{3/2}}{3}}}{2 \sqrt{\pi}\, x^{1/4}} + \frac{B\, e^{\frac{2 x^{3/2}}{3}}}{\sqrt{\pi}\, x^{1/4}}$

To satisfy the boundary condition $y(x) \to 0$ as $x \to +\infty$, we require $B = 0$, and therefore, the solution is, with $A = 1$,

$$y(x) = \mathrm{Ai}(x).$$

The solution with the proper boundary condition is immediately obtained using **SCWKBDSolve**:

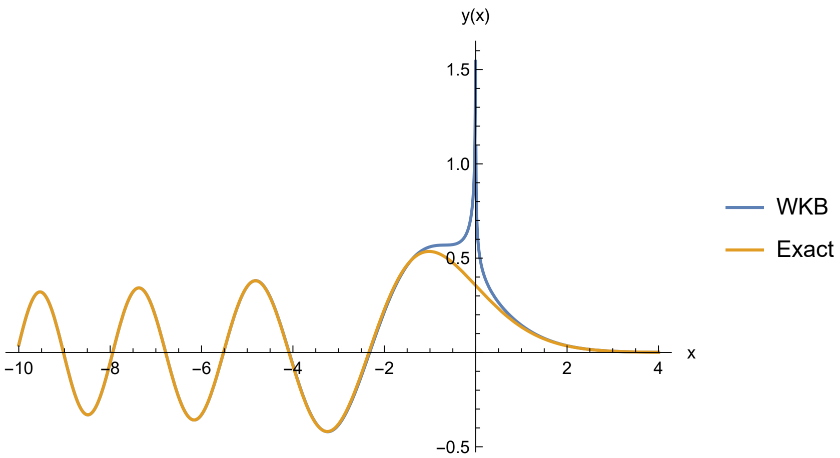
In[]:=
```
d²y/dx² - x y == 0
SCMAF[%, SCWKBDSolve,
 {All, y[x], {x, 0}, Evaluate → True, Connect → True}, Post → SCFuncShort,
 RA, {At[2], {C[1] → 1, C[2] → 0}}]
```

Out[]= $-x\,y + \frac{d^2 y}{dx^2} == 0$

$$y[x] == \begin{cases} \frac{1}{\sqrt{\pi}\,(-x)^{1/4}}\left(c_2 \operatorname{Cos}\left[\frac{\pi}{4} + \frac{2}{3}(-x)^{3/2}\right] + c_1 \operatorname{Sin}\left[\frac{\pi}{4} + \frac{2}{3}(-x)^{3/2}\right]\right) & x \ll 0 \\ \operatorname{Ai}[x]\, c_1 + \operatorname{Bi}[x]\, c_2 & x \approx 0 \\ \frac{1}{\sqrt{\pi}\,x^{1/4}}\left(\frac{1}{2} e^{-\frac{2x^{3/2}}{3}} c_1 + e^{\frac{2x^{3/2}}{3}} c_2\right) & x \gg 0 \\ 0 & \text{True} \end{cases}$$

Out[]=
$$y[x] == \begin{cases} \frac{1}{\sqrt{\pi}\,(-x)^{1/4}} \operatorname{Sin}\left[\frac{\pi}{4} + \frac{2}{3}(-x)^{3/2}\right] & x \ll 0 \\ \operatorname{Ai}[x] & x \approx 0 \\ \frac{e^{-\frac{2x^{3/2}}{3}}}{2\sqrt{\pi}\,x^{1/4}} & x \gg 0 \\ 0 & \text{True} \end{cases}$$

Plot of the WKB and exact solutions

Out[]=


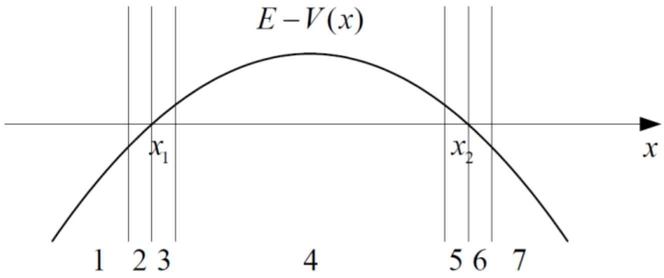
Bound States

Example 10

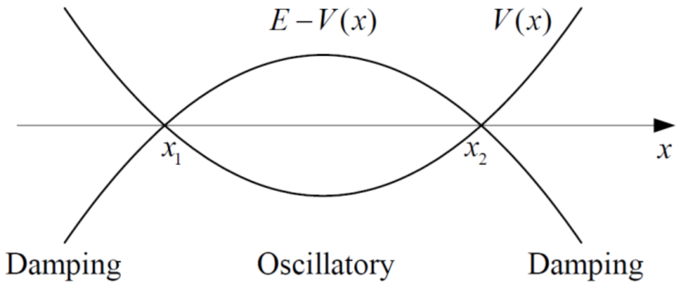
Solve the differential equation

$$\frac{d^2 u_E}{dx^2} + \frac{2m}{\hbar^2}(E - V(x))\,u_E = 0,$$

where E is the energy and $V(x)$ is the potential function.



The two points x_1 and x_2 are the turning points and the solution is oscillatory in the region $x_1 < x < x_2$ and exponentially decaying when $x \ll x_1$ and $x \gg x_2$.



The solution with the proper boundary conditions for $x \ll x_1$ and $x \gg x_2$ is immediately obtained using **SCWKBDSolve**:

In[∘]:=

```
d²u_E/dx² + (2 m/ℏ²) (E - V[x]) u_E == 0
SCMAF[%, SCWKBDSolve, {All, u_E, {x, x1, x2}, Assumptions → {m > 0, ℏ > 0, V′[x1] < 0, V′[x2] > 0},
  ReplVar → {x′, n}, ReplConst → {1, 0}, Connect → True, GenerateConditions → False},
 Post → {SCFuncShort, PowerExpand, SCChangeSign, {-m (E + _)/ℏ², E + _}},
 Hold → {-V′[x1]/V′[x2], -V′[x1]}]
```

Out[∘]= $\frac{d^2 u_E}{dx^2} + \frac{2\, m\, u_E\, (E - V[x])}{\hbar^2} == 0$

Out[∘]= $u_E == \begin{cases} \frac{(-1)^n e^{-\sqrt{2}\int_x^{x_1} \frac{\sqrt{m}\sqrt{-E+V[x']}}{\hbar} dx'} \sqrt{\hbar}}{2\times 2^{1/4} m^{1/4} \sqrt{\pi}\, (-E+V[x])^{1/4}} \left(-\frac{V'[x_1]}{V'[x_2]}\right)^{1/6} & x \ll x_1 \\ \frac{(-1)^n \hbar^{1/3}}{2^{1/6} m^{1/6} V'[x_2]^{1/6}} \mathrm{Ai}\left[\frac{2^{1/3} m^{1/3} (-x+x_1) (-V'[x_1])^{1/3}}{\hbar^{2/3}}\right] & x \approx x_1 \\ \frac{\sqrt{\hbar}}{2^{1/4} m^{1/4} \sqrt{\pi}\, (E-V[x])^{1/4}} \mathrm{Sin}\left[\frac{\pi}{4} + \sqrt{2}\int_x^{x_2} \frac{\sqrt{m}\sqrt{E-V[x']}}{\hbar} dx'\right] & x_1 \ll x \ll x_2 \\ \frac{\hbar^{1/3}}{2^{1/6} m^{1/6} V'[x_2]^{1/6}} \mathrm{Ai}\left[\frac{2^{1/3} m^{1/3} (x-x_2) V'[x_2]^{1/3}}{\hbar^{2/3}}\right] & x \approx x_2 \\ \frac{e^{-\sqrt{2}\int_{x_2}^{x} \frac{\sqrt{m}\sqrt{-E+V[x']}}{\hbar} dx'} \sqrt{\hbar}}{2\times 2^{1/4} m^{1/4} \sqrt{\pi}\, (-E+V[x])^{1/4}} & x \gg x_2 \\ 0 & \text{True} \end{cases}$

where

$$\sqrt{2} \int_{x_1}^{x_2} \sqrt{\frac{m\,(E - V(x'))}{\hbar^2}}\, dx' = \left(n + \frac{1}{2}\right)\pi, \quad n = 0, 1, 2, \ldots.$$

The classical turning points x_1 and x_2 are

In[ ]:=

```
E - V[x] == 0
SCMAF[%, RA, {All, V[x] == 1/2 m ω^2 x^2}, SCSolve → {x, ReplVar → {x1, x2}}, PowerMerge → True]
```

Out[ ]= $E - V[x] == 0$

Out[ ]= $\left\{x_1 == -\sqrt{2}\,\sqrt{\frac{E}{m}\frac{1}{\omega}},\ x_2 == \sqrt{2}\,\sqrt{\frac{E}{m}\frac{1}{\omega}}\right\}$

The energy eigenvalues are

In[ ]:=

```
√2 ∫_{x1}^{x2} Sqrt[m (E - V[x′]) / ℏ^2] dx′ == (1/2 + n) π
SCMAF[%, RA, {At[1], {V[x_] == 1/2 m ω^2 x^2, x1 == -√2 Sqrt[E/m 1/ω], x2 == √2 Sqrt[E/m 1/ω]}},
  Post → {SCIntSymmetrize, SCFactorInt, PowerExpand},
  SCEvalInt, At[1], RA → E == En, SCDivEq → {All, π/(ω ℏ)}, AddComment → "n = 0, 1, 2, ...."]
```

Out[ ]= $\sqrt{2}\int_{x_1}^{x_2}\sqrt{\frac{m\,(E - V[x'])}{\hbar^2}}\,dx' == \left(\frac{1}{2}+n\right)\pi$

$$\frac{2\sqrt{2}\,\sqrt{m}}{\hbar}\int_0^{\frac{\sqrt{2}\sqrt{E}}{\sqrt{m}\,\omega}}\sqrt{E - \frac{1}{2}m\,\omega^2\,x'^2}\,dx' == \left(\frac{1}{2}+n\right)\pi$$

$$E_n == \left(\frac{1}{2}+n\right)\omega\,\hbar$$

n = 0, 1, 2, ...

x_1 and x_2 are re-written in terms of $x_0 = \sqrt{\hbar/m\,\omega}$ as

In[ ]:=

```
{x1 == -√2 Sqrt[E/m 1/ω], x2 == √2 Sqrt[E/m 1/ω]}
SCMAF[%, RA, {All, E == (1/2 + n) ω ℏ}, PowerExpandMerge → True,
  RA → Sqrt[ℏ/(m ω)] == x0, Post → {SCPowerComb, {√2 Sqrt[1/2 + n], Post → Expand}}]
```

Out[ ]= $\left\{x_1 == -\sqrt{2}\,\sqrt{\frac{E}{m}\frac{1}{\omega}},\ x_2 == \sqrt{2}\,\sqrt{\frac{E}{m}\frac{1}{\omega}}\right\}$

Out[ ]= $\left\{x_1 == -\sqrt{1+2\,n}\,x_0,\ x_2 == \sqrt{1+2\,n}\,x_0\right\}$

The eigenfunction u_E is calculated as

In[•]:=

$$u_E == \begin{cases} \dfrac{(-1)^n e^{-\sqrt{2}\int_x^{x_1}\frac{\sqrt{m}\sqrt{-E+V[x']}}{\hbar}\,dx'}\sqrt{\hbar}}{2\times 2^{1/4} m^{1/4}\sqrt{\pi}\,(-E+V[x])^{1/4}}\left(-\dfrac{V'[x_1]}{V'[x_2]}\right)^{1/6} & x \ll x_1 \\ \dfrac{(-1)^n \hbar^{1/3}}{2^{1/6} m^{1/6} V'[x_2]^{1/6}}\,\mathrm{Ai}\left[\dfrac{2^{1/3} m^{1/3}(-x+x_1)(-V'[x_1])^{1/3}}{\hbar^{2/3}}\right] & x \approx x_1 \\ \dfrac{\sqrt{\hbar}}{2^{1/4} m^{1/4}\sqrt{\pi}\,(E-V[x])^{1/4}}\,\mathrm{Sin}\left[\dfrac{\pi}{4}+\sqrt{2}\int_x^{x_2}\dfrac{\sqrt{m}\sqrt{E-V[x']}}{\hbar}\,dx'\right] & x_1 \ll x \ll x_2 \\ \dfrac{\hbar^{1/3}}{2^{1/6} m^{1/6} V'[x_2]^{1/6}}\,\mathrm{Ai}\left[\dfrac{2^{1/3} m^{1/3}(x-x_2)V'[x_2]^{1/3}}{\hbar^{2/3}}\right] & x \approx x_2 \\ \dfrac{e^{-\sqrt{2}\int_{x_2}^{x}\frac{\sqrt{m}\sqrt{-E+V[x']}}{\hbar}\,dx'}\sqrt{\hbar}}{2\times 2^{1/4} m^{1/4}\sqrt{\pi}\,(-E+V[x])^{1/4}} & x \gg x_2 \\ 0 & \text{True} \end{cases};$$

$$\text{SCMAF}\Big[\%,\ \text{SCFuncRA},$$

$$\left\{\text{At}[2],\ \left\{V[x\_] \to \frac{1}{2} m\,\omega^2 x^2,\ E == \left(\frac{1}{2}+n\right)\omega\,\hbar,\ x_1 == -\sqrt{1+2n}\,x_0,\ x_2 == \sqrt{1+2n}\,x_0\right\}\right\},$$

$$\text{Post} \to \Big\{\text{SCFactorInt, PowerExpand, SCFactor},\ \{\hbar\,\omega\,\_ + \_,\ \hbar\,\omega\},$$

$$\text{PowerExpand, SCEliminate} \to \left\{\sqrt{\frac{\hbar}{m\,\omega}} == x_0,\ m\right\}\Big\},\ \text{Quiet} \to \text{True},$$

$$\text{SCTransInt},\ \left\{\text{At}[2],\ \text{TransVar} \to \left\{x',\ t,\ t == \frac{x'}{\sqrt{2}\,x_0}\right\}\right\},\ \text{Post} \to \text{SCFactorInt},$$

$$\text{SCEvalInt},\ \left\{\int_{\frac{x}{\sqrt{2}\,x_0}}^{-\frac{\sqrt{1+2n}}{\sqrt{2}}} \sqrt{-\frac{1}{2} - n + t^2}\,dt,\ \text{Assumptions} \to \{n \in \mathbb{Z},\ n \geq 0,\ x_0 > 0,\ x < 0\}\right\},$$

$$\text{SCEvalInt},\ \left\{\int_{\frac{x}{\sqrt{2}\,x_0}}^{\frac{\sqrt{1+2n}}{\sqrt{2}}} \sqrt{\frac{1}{2} + n - t^2}\,dt,\ \text{Assumptions} \to \{n \in \mathbb{Z},\ n \geq 0,\ x_0 > 0,\ -x_0 < x < x_0\}\right\},$$

$$\text{SCEvalInt},\ \left\{\int_{\frac{\sqrt{1+2n}}{\sqrt{2}}}^{\frac{x}{\sqrt{2}\,x_0}} \sqrt{-\frac{1}{2} - n + t^2}\,dt,\ \text{Assumptions} \to \{n \in \mathbb{Z},\ n \geq 0,\ x_0 > 0,\ x > 0\}\right\},\ ,\ ,$$

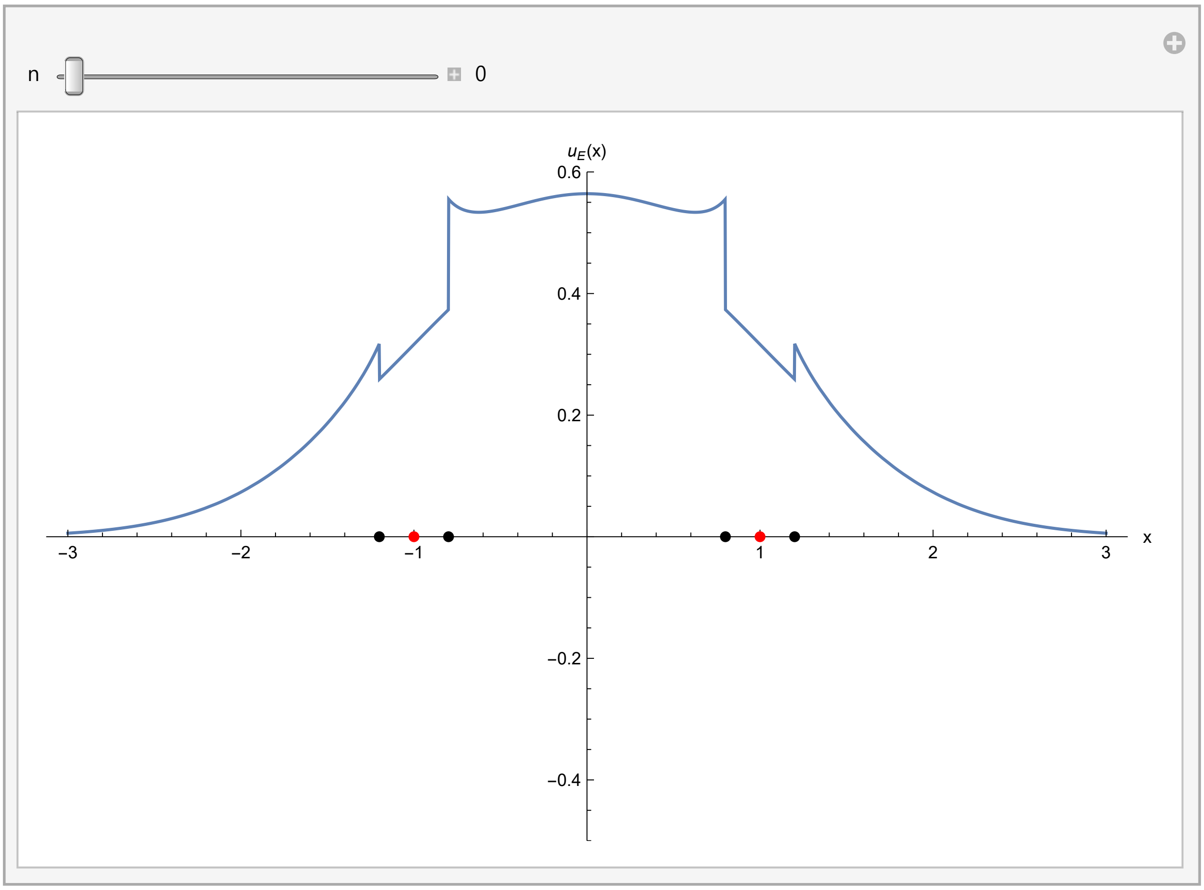
$$\text{SCIfTrue, All}\Big]$$

Out[•]=

$$u_E == \begin{cases} \dfrac{(-1)^n e^{\frac{1}{4}\left(-(1+2n)\left(\mathrm{Log}[1+2n]-2\,\mathrm{Log}\left[\frac{-x+\sqrt{x^2-(1+2n)x_0^2}}{x_0}\right]\right)+\frac{2x}{x_0}\sqrt{-1-2n+\frac{x^2}{x_0^2}}\right)}\sqrt{x_0}}{2\times 2^{1/4}\sqrt{\pi}\left(-\frac{1}{2}-n+\frac{x^2}{2x_0^2}\right)^{1/4}} & x \ll -\sqrt{1+2n}\,x_0 \\ \dfrac{(-1)^n\sqrt{x_0}}{2^{1/6}(1+2n)^{1/12}}\,\mathrm{Ai}\left[\dfrac{2^{1/3}(1+2n)^{1/6}\left(-x-\sqrt{1+2n}\,x_0\right)}{x_0}\right] & x \approx -\sqrt{1+2n}\,x_0 \\ \dfrac{\sqrt{x_0}\,\mathrm{Sin}\left[\frac{\pi}{4}+\frac{1}{4}\times\left((1+2n)\left(\pi-2\,\mathrm{ArcTan}\left[\frac{x}{\sqrt{-x^2+(1+2n)x_0^2}}\right]\right)-\frac{2x}{x_0}\sqrt{1+2n-\frac{x^2}{x_0^2}}\right)\right]}{2^{1/4}\sqrt{\pi}\left(\frac{1}{2}+n-\frac{x^2}{2x_0^2}\right)^{1/4}} & -\sqrt{1+2n}\,x_0 \ll x \ll \sqrt{1+2n}\,x_0 \\ \dfrac{\sqrt{x_0}}{2^{1/6}(1+2n)^{1/12}}\,\mathrm{Ai}\left[\dfrac{2^{1/3}(1+2n)^{1/6}\left(x-\sqrt{1+2n}\,x_0\right)}{x_0}\right] & x \approx \sqrt{1+2n}\,x_0 \\ \dfrac{e^{\frac{1}{4}\left(-(1+2n)\left(\mathrm{Log}[1+2n]-2\,\mathrm{Log}\left[\frac{x+\sqrt{x^2-(1+2n)x_0^2}}{x_0}\right]\right)-\frac{2x}{x_0}\sqrt{-1-2n+\frac{x^2}{x_0^2}}\right)}\sqrt{x_0}}{2\times 2^{1/4}\sqrt{\pi}\left(-\frac{1}{2}-n+\frac{x^2}{2x_0^2}\right)^{1/4}} & x \gg \sqrt{1+2n}\,x_0 \\ 0 & \text{True} \end{cases}$$

Plot of u_E with n as the parameter

Out[ ]=



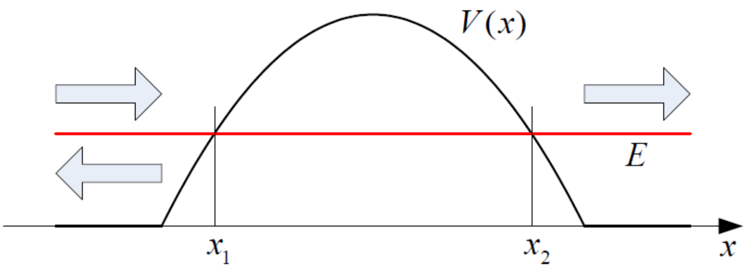
Tunneling

Example 11

Solve the differential equation

$$\frac{d^2 u}{d x^2} + \frac{2\, m}{\hbar^2} (E - V(x))\, u = 0, \quad E < V_{\max},$$

where E is the energy and $V(x)$ is the potential function.



The two points x_1 and x_2 are the classical turning points and the solution is exponential in the region $x_1 < x < x_2$ and oscillatory where $x \ll x_1$ and $x \gg x_2$. We assume that the wave is incident from the left side with energy E. We will calculate the reflectivity and transmittivity due to the presence of the potential $V(x)$.

The solution is immediately obtained using **SCWKBDSolve**:

In[∘]:=
```
d²u/dx² + 2m/ℏ² (E - V[x]) u == 0
SCMAF[%, SCWKBDSolve, {All, u, {x, x1, x2}, Assumptions → {m > 0, ℏ > 0, V′[x1] > 0, V′[x2] < 0},
  ReplVar → x′, Connect → True, Reference → x2}, Post → SCFuncShort]
```

Out[∘]= $\frac{d^2u}{dx^2} + \frac{2\,m\,u\,(E - V[x])}{\hbar^2} == 0$

Out[∘]= $u == \begin{cases} \frac{\left(-\frac{V'[x_1]}{V'[x_2]}\right)^{1/6}}{2^{1/4}\sqrt{\pi}\left(\frac{m(E-V[x])}{\hbar^2}\right)^{1/4}}\left(\frac{1}{2} e^{-\sqrt{2}\int_{x_1}^{x_2}\sqrt{-\frac{m(E-V[x'])}{\hbar^2}}\,dx'} c_1 \mathrm{Cos}\left[\frac{\pi}{4} + \sqrt{2}\int_x^{x_1}\sqrt{\frac{m(E-V[x'])}{\hbar^2}}\,dx'\right] + 2 e^{\sqrt{2}\int_{x_1}^{x_2}\sqrt{-\frac{m(E-V[x'])}{\hbar^2}}\,dx'} c_2 \mathrm{Sin}\left[\frac{\pi}{4} + \sqrt{2}\int_x^{x_1}\sqrt{\frac{m(E-V[x'])}{\hbar^2}}\,dx'\right]\right) & x \ll x_1 \\ \frac{\frac{1}{2} e^{-\sqrt{2}\int_{x_1}^{x_2}\sqrt{-\frac{m(E-V[x'])}{\hbar^2}}\,dx'} c_1 \mathrm{Bi}\left[2^{1/3}\left(\frac{m V'[x_1]}{\hbar^2}\right)^{1/3}(x-x_1)\right] + 2 e^{\sqrt{2}\int_{x_1}^{x_2}\sqrt{-\frac{m(E-V[x'])}{\hbar^2}}\,dx'} c_2 \mathrm{Ai}\left[2^{1/3}\left(\frac{m V'[x_1]}{\hbar^2}\right)^{1/3}(x-x_1)\right]}{2^{1/6}\left(-\frac{m V'[x_2]}{\hbar^2}\right)^{1/6}} & x \approx x_1 \\ \frac{\frac{1}{2} e^{-\sqrt{2}\int_x^{x_2}\sqrt{-\frac{m(E-V[x'])}{\hbar^2}}\,dx'} c_1 + e^{\sqrt{2}\int_x^{x_2}\sqrt{-\frac{m(E-V[x'])}{\hbar^2}}\,dx'} c_2}{2^{1/4}\sqrt{\pi}\left(-\frac{m(E-V[x])}{\hbar^2}\right)^{1/4}} & x_1 \ll x \\ \frac{c_1 \mathrm{Ai}\left[2^{1/3}\left(-\frac{m V'[x_2]}{\hbar^2}\right)^{1/3}(-x+x_2)\right] + c_2 \mathrm{Bi}\left[2^{1/3}\left(-\frac{m V'[x_2]}{\hbar^2}\right)^{1/3}(-x+x_2)\right]}{2^{1/6}\left(-\frac{m V'[x_2]}{\hbar^2}\right)^{1/6}} & x \approx x_2 \\ \frac{1}{2^{1/4}\sqrt{\pi}\left(\frac{m(E-V[x])}{\hbar^2}\right)^{1/4}}\left(c_2 \mathrm{Cos}\left[\frac{\pi}{4} + \sqrt{2}\int_{x_2}^{x}\sqrt{\frac{m(E-V[x'])}{\hbar^2}}\,dx'\right] + c_1 \mathrm{Sin}\left[\frac{\pi}{4} + \sqrt{2}\int_{x_2}^{x}\sqrt{\frac{m(E-V[x'])}{\hbar^2}}\,dx'\right]\right) & x \gg x_2 \\ 0 & \mathrm{True} \end{cases}$

The arbitrary constants c_1 and c_2 are to be determined to satisfy the proper boundary conditions for $x \ll x_1$ and $x \gg x_2$.

In the region $x \gg x_2$, let us put

In[∘]:=
```
v3 == c2 Cos[π/4 + √2 ∫_{x2}^{x} √(m (E - V[x′])/ℏ²) dx′] + c1 Sin[π/4 + √2 ∫_{x2}^{x} √(m (E - V[x′])/ℏ²) dx′];
SCMAF[%, TrigExpand, At[2], Post → TrigToExp,
 Collect, {At[2], {e^(i √2 ∫_{x2}^{x} √(m (E-V[x′])/ℏ²) dx′), e^(-i √2 ∫_{x2}^{x} √(m (E-V[x′])/ℏ²) dx′)}, Simplify}]
```

$$v_3 == \frac{\left(\frac{1}{2}+\frac{i}{2}\right) e^{-i\sqrt{2}\int_{x_2}^{x}\sqrt{\frac{m(E-V[x'])}{\hbar^2}}\,dx'} c_1}{\sqrt{2}} + \frac{\left(\frac{1}{2}-\frac{i}{2}\right) e^{i\sqrt{2}\int_{x_2}^{x}\sqrt{\frac{m(E-V[x'])}{\hbar^2}}\,dx'} c_1}{\sqrt{2}} + \frac{\left(\frac{1}{2}-\frac{i}{2}\right) e^{-i\sqrt{2}\int_{x_2}^{x}\sqrt{\frac{m(E-V[x'])}{\hbar^2}}\,dx'} c_2}{\sqrt{2}} + \frac{\left(\frac{1}{2}+\frac{i}{2}\right) e^{i\sqrt{2}\int_{x_2}^{x}\sqrt{\frac{m(E-V[x'])}{\hbar^2}}\,dx'} c_2}{\sqrt{2}}$$

Out[∘]= $v_3 == \frac{\left(\frac{1}{2}+\frac{i}{2}\right) e^{-i\sqrt{2}\int_{x_2}^{x}\sqrt{\frac{m(E-V[x'])}{\hbar^2}}\,dx'} (c_1 - i\,c_2)}{\sqrt{2}} + \frac{\left(\frac{1}{2}+\frac{i}{2}\right) e^{i\sqrt{2}\int_{x_2}^{x}\sqrt{\frac{m(E-V[x'])}{\hbar^2}}\,dx'} (-i\,c_1 + c_2)}{\sqrt{2}}$

Since only the transmitted wave exists in the far right side, the arbitrary constants c_1 and c_2 are determined as

In[∘]:=

```
SCSolve[{c1 - i c2 == 0, ((1/2 + i/2) (-i c1 + c2))/Sqrt[2] == 1}, {c1, c2}]
```

Out[∘]=

$$\left\{c_1 == \frac{1+i}{\sqrt{2}},\ c_2 == \frac{1-i}{\sqrt{2}}\right\}$$

which gives

In[∘]:=

```
v3 == ((1/2 + i/2) e^(-i Sqrt[2] ∫_{x2}^{x} Sqrt[m (E - V[x'])/ħ^2] dx') (c1 - i c2))/Sqrt[2] + ((1/2 + i/2) e^(i Sqrt[2] ∫_{x2}^{x} Sqrt[m (E - V[x'])/ħ^2] dx') (-i c1 + c2))/Sqrt[2];
SCMAF[%, RA, {At[2], {c1 == (1 + i)/Sqrt[2], c2 == (1 - i)/Sqrt[2]}}]
```

Out[∘]=

$$v_3 == e^{i\sqrt{2}\int_{x_2}^{x}\sqrt{\frac{m(E-V[x'])}{\hbar^2}}\,dx'}$$

In the region $x \ll x_1$, we then have

In[∘]:=

```
v1 == 1/2 e^(-Sqrt[2] ∫_{x1}^{x2} Sqrt[-m (E - V[x'])/ħ^2] dx') c1 Cos[π/4 + Sqrt[2] ∫_{x}^{x1} Sqrt[m (E - V[x'])/ħ^2] dx'] +
   2 e^(Sqrt[2] ∫_{x1}^{x2} Sqrt[-m (E - V[x'])/ħ^2] dx') c2 Sin[π/4 + Sqrt[2] ∫_{x}^{x1} Sqrt[m (E - V[x'])/ħ^2] dx'];
SCMAF[%, RA, {At[2], {c1 == (1 + i)/Sqrt[2], c2 == (1 - i)/Sqrt[2]}}, Post → {TrigToExp, TrigExpand},
  Collect, {At[2], {e^(i Sqrt[2] ∫_{x}^{x1} Sqrt[m (E - V[x'])/ħ^2] dx'), e^(-i Sqrt[2] ∫_{x}^{x1} Sqrt[m (E - V[x'])/ħ^2] dx')}}]
```

$$v_1 == \frac{1}{4}e^{-\sqrt{2}\int_{x_1}^{x_2}\sqrt{-\frac{m(E-V[x'])}{\hbar^2}}\,dx'-i\sqrt{2}\int_{x}^{x_1}\sqrt{\frac{m(E-V[x'])}{\hbar^2}}\,dx'}+e^{\sqrt{2}\int_{x_1}^{x_2}\sqrt{-\frac{m(E-V[x'])}{\hbar^2}}\,dx'-i\sqrt{2}\int_{x}^{x_1}\sqrt{\frac{m(E-V[x'])}{\hbar^2}}\,dx'}+$$
$$\frac{1}{4}\,i\,e^{-\sqrt{2}\int_{x_1}^{x_2}\sqrt{-\frac{m(E-V[x'])}{\hbar^2}}\,dx'+i\sqrt{2}\int_{x}^{x_1}\sqrt{\frac{m(E-V[x'])}{\hbar^2}}\,dx'}-i\,e^{\sqrt{2}\int_{x_1}^{x_2}\sqrt{-\frac{m(E-V[x'])}{\hbar^2}}\,dx'+i\sqrt{2}\int_{x}^{x_1}\sqrt{\frac{m(E-V[x'])}{\hbar^2}}\,dx'}$$

Out[∘]=

$$v_1 == e^{i\sqrt{2}\int_{x}^{x_1}\sqrt{\frac{m(E-V[x'])}{\hbar^2}}\,dx'}\left(\frac{1}{4}\,i\,e^{-\sqrt{2}\int_{x_1}^{x_2}\sqrt{-\frac{m(E-V[x'])}{\hbar^2}}\,dx'}-i\,e^{\sqrt{2}\int_{x_1}^{x_2}\sqrt{-\frac{m(E-V[x'])}{\hbar^2}}\,dx'}\right)+$$
$$e^{-i\sqrt{2}\int_{x}^{x_1}\sqrt{\frac{m(E-V[x'])}{\hbar^2}}\,dx'}\left(\frac{1}{4}e^{-\sqrt{2}\int_{x_1}^{x_2}\sqrt{-\frac{m(E-V[x'])}{\hbar^2}}\,dx'}+e^{\sqrt{2}\int_{x_1}^{x_2}\sqrt{-\frac{m(E-V[x'])}{\hbar^2}}\,dx'}\right)$$

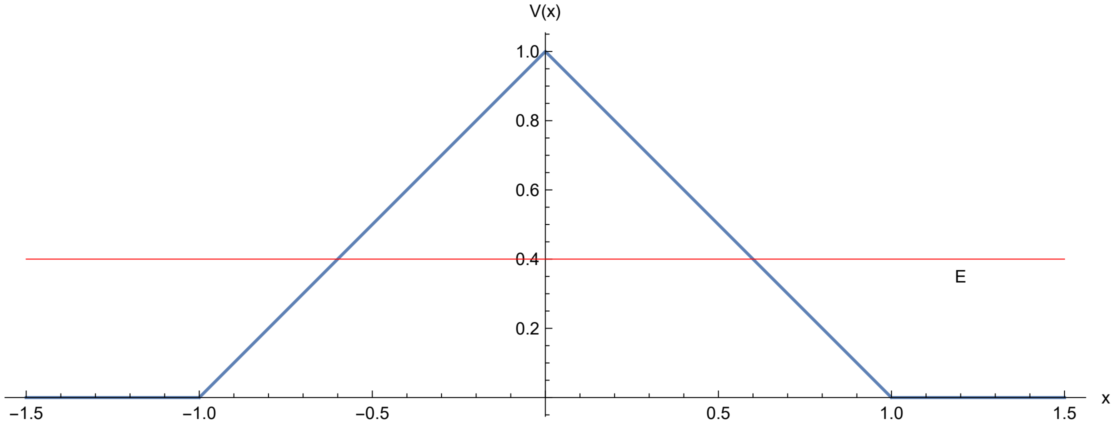
The solutions u_1 ($x \ll x_1$) and u_3 ($x \gg x_2$) are given by

In[∘]:=
```
{u1 == (-V'[x1]/V'[x2])^(1/6) / (2^(1/4) Sqrt[π] (m (E-V[x])/ℏ^2)^(1/4)) v1, u3 == 1/(2^(1/4) Sqrt[π] (m (E-V[x])/ℏ^2)^(1/4)) v3} /. V[x] → 0;
SCMAF[%, SCRecipPower, (m E/ℏ^2)^(1/4)]
```

Out[∘]= $\left\{u_1 == \frac{1}{2^{1/4}\sqrt{\pi}}\left(\frac{\hbar^2}{m E}\right)^{1/4}\left(-\frac{V'[x_1]}{V'[x_2]}\right)^{1/6} v_1,\ u_3 == \frac{1}{2^{1/4}\sqrt{\pi}}\left(\frac{\hbar^2}{m E}\right)^{1/4} v_3\right\}$

As an example, let us suppose the potential $V(x)$ is given by

$$V(x) = \begin{cases} V_0(1-|x|) & -1 < x < 1 \\ 0 & \text{otherwise} \end{cases}, \quad 0 < E < V_0.$$

Out[∘]=


The classical turning points x_1 and x_2 are

In[∘]:=
```
E - V[x] == 0
SCMAF[%, RA, {All, V[x] == V0 (1 - |x|)}, SCSolve → {x, Post → Expand, ReplVar → {x1, x2}}]
```

Out[∘]= $E - V[x] == 0$

Out[∘]= $\left\{x_1 == -1 + \frac{E}{V_0},\ x_2 == 1 - \frac{E}{V_0}\right\}$

Evaluating the integrals, the solutions u_1 and u_3 are given as

In[ ]:=

$$\left\{u_1 == \frac{1}{2^{1/4}\sqrt{\pi}}\left(\frac{\hbar^2}{m\,E}\right)^{1/4}\left(-\frac{V'[x_1]}{V'[x_2]}\right)^{1/6} v_1,\ u_3 == \frac{1}{2^{1/4}\sqrt{\pi}}\left(\frac{\hbar^2}{m\,E}\right)^{1/4} v_3\right\}$$

$$\text{SCMAF}\Big[\%,\ \text{RA},\ \Big\{\text{At}[1],\ \frac{V'[x_1]}{V'[x_2]} == -1\Big\},$$

$$\text{RA},\ \Big\{\text{All},\ \Big\{v_1 == e^{i\sqrt{2}\int_x^{x_1}\sqrt{\frac{m(E-V[x'])}{\hbar^2}}\,dx'}\left(\frac{1}{4}\,i\,e^{-\sqrt{2}\int_{x_1}^{x_2}\sqrt{\frac{m(-E+V[x'])}{\hbar^2}}\,dx'} - i\,e^{\sqrt{2}\int_{x_1}^{x_2}\sqrt{\frac{m(-E+V[x'])}{\hbar^2}}\,dx'}\right) +$$

$$e^{-i\sqrt{2}\int_x^{x_1}\sqrt{\frac{m(E-V[x'])}{\hbar^2}}\,dx'}\left(\frac{1}{4}\,e^{-\sqrt{2}\int_{x_1}^{x_2}\sqrt{\frac{m(-E+V[x'])}{\hbar^2}}\,dx'} + e^{\sqrt{2}\int_{x_1}^{x_2}\sqrt{\frac{m(-E+V[x'])}{\hbar^2}}\,dx'}\right),\ v_3 == e^{i\sqrt{2}\int_{x_2}^{x}\sqrt{\frac{m(E-V[x'])}{\hbar^2}}\,dx'}\Big\}\Big\},$$

$$\text{SCIntChangeInterval},\ \Big\{\Big\{\int_x^{x_1} f\_\,dx',\ \{x',\ \{x,\ -1,\ V[x\_] == 0\},\ \{-1,\ x_1,\ V[x\_] == V_0\,(1+x)\}\}\Big\},$$

$$\Big\{\int_{x_1}^{x_2} f\_\,dx',\ \{x',\ \{x_1,\ 0,\ V[x\_] == V_0\,(1+x)\},\ \{0,\ x_2,\ V[x\_] == V_0\,(1-x)\}\}\Big\},$$

$$\Big\{\int_{x_2}^{x} f\_\,dx',\ \{x',\ \{x_2,\ 1,\ V[x\_] == V_0\,(1-x)\},\ \{1,\ x,\ V[x\_] == 0\}\}\Big\}\Big\},$$

$$\text{SCEvalInt},\ \{\text{All},\ \text{GenerateConditions} \to \text{False}\},$$

$$\text{RA},\ \Big\{\text{All},\ \Big\{x_1 == -1 + \frac{E}{V_0},\ x_2 == 1 - \frac{E}{V_0}\Big\}\Big\},$$

$$\text{SCExpandExp},\ \text{At}[\_,\ 2],\ \text{Post} \to \text{Expand},$$

$$\text{SCEliminate},\ \Big\{\text{At}[\_,\ 2],\ \Big\{k == \sqrt{\frac{2\,m\,E}{\hbar^2}},\ \epsilon == \frac{E}{V_0}\Big\},\ \{E,\ V_0\}\Big\},\ \text{Quiet} \to \text{True},$$

$$\text{Simplify},\ \text{At}[\_,\ 2],\ \text{ChangeSign} \to -1 + \_,\ \text{Post} \to \{\text{ExpandAll},\ \text{PowerExpand}\},$$

$$\text{Collect},\ \Big\{\text{At}[1,\ 2],\ \{e^{i k x},\ e^{-i k x}\},\ \text{SCFactor}\Big[\#,\ \frac{1}{\sqrt{k}\,\sqrt{\pi}}\Big]\&\Big\}\Big]$$

Out[ ]=

$$\left\{u_1 == \frac{1}{2^{1/4}\sqrt{\pi}}\left(\frac{\hbar^2}{m\,E}\right)^{1/4}\left(-\frac{V'[x_1]}{V'[x_2]}\right)^{1/6} v_1,\ u_3 == \frac{1}{2^{1/4}\sqrt{\pi}}\left(\frac{\hbar^2}{m\,E}\right)^{1/4} v_3\right\}$$

$$\Big\{u_1 == \frac{e^{i k + i k x + \frac{4k\sqrt{1-\epsilon}}{3\sqrt{\epsilon}} - \frac{4}{3}k\sqrt{1-\epsilon}\,\sqrt{\epsilon} - \frac{2 i k \epsilon}{3}}}{\sqrt{k}\,\sqrt{\pi}} + \frac{e^{i k + i k x - \frac{4k\sqrt{1-\epsilon}}{3\sqrt{\epsilon}} + \frac{4}{3}k\sqrt{1-\epsilon}\,\sqrt{\epsilon} - \frac{2 i k \epsilon}{3}}}{4\sqrt{k}\,\sqrt{\pi}} -$$

$$\frac{i\,e^{-i k - i k x + \frac{4k\sqrt{1-\epsilon}}{3\sqrt{\epsilon}} - \frac{4}{3}k\sqrt{1-\epsilon}\,\sqrt{\epsilon} + \frac{2 i k \epsilon}{3}}}{\sqrt{k}\,\sqrt{\pi}} + \frac{i\,e^{-i k - i k x - \frac{4k\sqrt{1-\epsilon}}{3\sqrt{\epsilon}} + \frac{4}{3}k\sqrt{1-\epsilon}\,\sqrt{\epsilon} + \frac{2 i k \epsilon}{3}}}{4\sqrt{k}\,\sqrt{\pi}},\ u_3 == \frac{e^{-i k + i k x + \frac{2 i k \epsilon}{3}}}{\sqrt{k}\,\sqrt{\pi}}\Big\}$$

Out[ ]=

$$\Big\{u_1 == \frac{e^{i k x}}{\sqrt{k}\,\sqrt{\pi}}\left(e^{i k + \frac{4k\sqrt{1-\epsilon}}{3\sqrt{\epsilon}} - \frac{4}{3}k\sqrt{1-\epsilon}\,\sqrt{\epsilon} - \frac{2 i k \epsilon}{3}} + \frac{1}{4}\,e^{i k - \frac{4k\sqrt{1-\epsilon}}{3\sqrt{\epsilon}} + \frac{4}{3}k\sqrt{1-\epsilon}\,\sqrt{\epsilon} - \frac{2 i k \epsilon}{3}}\right) +$$

$$\frac{e^{-i k x}}{\sqrt{k}\,\sqrt{\pi}}\left(-i\,e^{-i k + \frac{4k\sqrt{1-\epsilon}}{3\sqrt{\epsilon}} - \frac{4}{3}k\sqrt{1-\epsilon}\,\sqrt{\epsilon} + \frac{2 i k \epsilon}{3}} + \frac{1}{4}\,i\,e^{-i k - \frac{4k\sqrt{1-\epsilon}}{3\sqrt{\epsilon}} + \frac{4}{3}k\sqrt{1-\epsilon}\,\sqrt{\epsilon} + \frac{2 i k \epsilon}{3}}\right),\ u_3 == \frac{e^{-i k + i k x + \frac{2 i k \epsilon}{3}}}{\sqrt{k}\,\sqrt{\pi}}\Big\}$$

where

$$k = \sqrt{\frac{2\,m\,E}{\hbar^2}}\,, \quad \epsilon = \frac{E}{V_0}.$$

The reflection and transmission coefficients are

In[∘]:=

$$\left\{r == \frac{-i\, e^{-i k+\frac{4 k \sqrt{1-\epsilon}}{3 \sqrt{\epsilon}}-\frac{4}{3} k \sqrt{1-\epsilon} \sqrt{\epsilon}+\frac{2 i k \epsilon}{3}}+\frac{1}{4} i\, e^{-i k-\frac{4 k \sqrt{1-\epsilon}}{3 \sqrt{\epsilon}}+\frac{4}{3} k \sqrt{1-\epsilon} \sqrt{\epsilon}+\frac{2 i k \epsilon}{3}}}{e^{i k+\frac{4 k \sqrt{1-\epsilon}}{3 \sqrt{\epsilon}}-\frac{4}{3} k \sqrt{1-\epsilon} \sqrt{\epsilon}-\frac{2 i k \epsilon}{3}}+\frac{1}{4} e^{i k-\frac{4 k \sqrt{1-\epsilon}}{3 \sqrt{\epsilon}}+\frac{4}{3} k \sqrt{1-\epsilon} \sqrt{\epsilon}-\frac{2 i k \epsilon}{3}}},\right.$$

$$\left. t == \frac{e^{-i k+\frac{2 i k \epsilon}{3}}}{e^{i k+\frac{4 k \sqrt{1-\epsilon}}{3 \sqrt{\epsilon}}-\frac{4}{3} k \sqrt{1-\epsilon} \sqrt{\epsilon}-\frac{2 i k \epsilon}{3}}+\frac{1}{4} e^{i k-\frac{4 k \sqrt{1-\epsilon}}{3 \sqrt{\epsilon}}+\frac{4}{3} k \sqrt{1-\epsilon} \sqrt{\epsilon}-\frac{2 i k \epsilon}{3}}}\right\};$$

```
SCMAF[%, Simplify, At[_, 2], ChangeSign → -1 + _, PowerFullMerge → True]
```

Out[∘]=

$$\left\{r == -\frac{i\, e^{\frac{2}{3} i k (-3+2 \epsilon)}\left(4 e^{\frac{8 k}{3}\sqrt{\frac{1-\epsilon}{\epsilon}}}-e^{\frac{8}{3} k \sqrt{(1-\epsilon) \epsilon}}\right)}{4 e^{\frac{8 k}{3}\sqrt{\frac{1-\epsilon}{\epsilon}}}+e^{\frac{8}{3} k \sqrt{(1-\epsilon) \epsilon}}},\ t == \frac{4 e^{\frac{2 k}{3}\left(-3 i+2 \sqrt{\frac{1-\epsilon}{\epsilon}}+2 i \epsilon+2 \sqrt{(1-\epsilon) \epsilon}\right)}}{4 e^{\frac{8 k}{3}\sqrt{\frac{1-\epsilon}{\epsilon}}}+e^{\frac{8}{3} k \sqrt{(1-\epsilon) \epsilon}}}\right\}$$

The reflectivity and transmittivity are

In[∘]:=

$$\{R == |r|^2,\ T == |t|^2\}$$

SCMAF[%, RA,

$$\left\{All, \left\{r == -\frac{i\, e^{\frac{2}{3} i k (-3+2 \epsilon)}\left(4 e^{\frac{8 k}{3}\sqrt{\frac{1-\epsilon}{\epsilon}}}-e^{\frac{8}{3} k \sqrt{(1-\epsilon) \epsilon}}\right)}{4 e^{\frac{8 k}{3}\sqrt{\frac{1-\epsilon}{\epsilon}}}+e^{\frac{8}{3} k \sqrt{(1-\epsilon) \epsilon}}},\ t == \frac{4 e^{\frac{2 k}{3}\left(-3 i+2 \sqrt{\frac{1-\epsilon}{\epsilon}}+2 i \epsilon+2 \sqrt{(1-\epsilon) \epsilon}\right)}}{4 e^{\frac{8 k}{3}\sqrt{\frac{1-\epsilon}{\epsilon}}}+e^{\frac{8}{3} k \sqrt{(1-\epsilon) \epsilon}}}\right\}\right\},$$

SCComplexExpand, All, ChangeSign → $-1+\epsilon$,

Post → {PowerFullMerge → True, Together, $-1+\frac{1}{\epsilon}$, PowerExpand},

SCDivFrac, {All, $16\, e^{\frac{16 k}{3}\sqrt{\frac{1-\epsilon}{\epsilon}}}$, Positive → True}, Hold → $\frac{1-\epsilon}{\epsilon}$,

Post → {SCFactorExp → $-\frac{8 k}{3}$, SCExpandExp},

RA, {All, $-\frac{8 k}{3}\left(\sqrt{\frac{1-\epsilon}{\epsilon}}-\sqrt{(1-\epsilon) \epsilon}\right) == -\xi$}]

Out[∘]=

$$\{R == |r|^2,\ T == |t|^2\}$$

$$\left\{R == \frac{\left(1-\frac{1}{4} e^{-\frac{8 k}{3}\left(\sqrt{\frac{1-\epsilon}{\epsilon}}-\sqrt{(1-\epsilon) \epsilon}\right)}\right)^2}{\left(1+\frac{1}{4} e^{-\frac{8 k}{3}\left(\sqrt{\frac{1-\epsilon}{\epsilon}}-\sqrt{(1-\epsilon) \epsilon}\right)}\right)^2},\ T == \frac{e^{-\frac{8 k}{3}\left(\sqrt{\frac{1-\epsilon}{\epsilon}}-\sqrt{(1-\epsilon) \epsilon}\right)}}{\left(1+\frac{1}{4} e^{-\frac{8 k}{3}\left(\sqrt{\frac{1-\epsilon}{\epsilon}}-\sqrt{(1-\epsilon) \epsilon}\right)}\right)^2}\right\}$$

Out[∘]=

$$\left\{R == \frac{\left(1-\frac{e^{-\xi}}{4}\right)^2}{\left(1+\frac{e^{-\xi}}{4}\right)^2},\ T == \frac{e^{-\xi}}{\left(1+\frac{e^{-\xi}}{4}\right)^2}\right\}$$

where

$$\xi = \frac{8 k}{3}\left(\sqrt{\frac{1-\epsilon}{\epsilon}}-\sqrt{(1-\epsilon) \epsilon}\right), \quad k=\sqrt{\frac{2 m E}{\hbar^2}}, \quad \epsilon=\frac{E}{V_0}.$$

The sum $R+T$ is equal to 1.

In[∘]:=
$$\text{SCARA}\left[R+T,\ \left\{R==\frac{\left(1-\frac{e^{-\xi}}{4}\right)^2}{\left(1+\frac{e^{-\xi}}{4}\right)^2},\ T==\frac{e^{-\xi}}{\left(1+\frac{e^{-\xi}}{4}\right)^2}\right\},\ \text{Post}\to\text{Simplify}\right]$$

Out[∘]= R + T == 1

For small energy ($\epsilon \ll 1$), $\xi \gg 1$ and $e^{-\xi} \ll 1$. This gives

In[∘]:=
$$\left\{R==\frac{\left(1-\frac{e^{-\xi}}{4}\right)^2}{\left(1+\frac{e^{-\xi}}{4}\right)^2},\ T==\frac{e^{-\xi}}{\left(1+\frac{e^{-\xi}}{4}\right)^2}\right\}$$

```
SCMAF[%, SCTaylorSeries, {At[_, 2], e^-ξ}, Head → TildeTilde]
```

Out[∘]=
$$\left\{R==\frac{\left(1-\frac{e^{-\xi}}{4}\right)^2}{\left(1+\frac{e^{-\xi}}{4}\right)^2},\ T==\frac{e^{-\xi}}{\left(1+\frac{e^{-\xi}}{4}\right)^2}\right\}$$

Out[∘]= $\left\{R \approx 1-e^{-\xi},\ T \approx e^{-\xi}\right\}$

For large energy ($\epsilon \lesssim 1$), $\xi \approx 0$, and we have

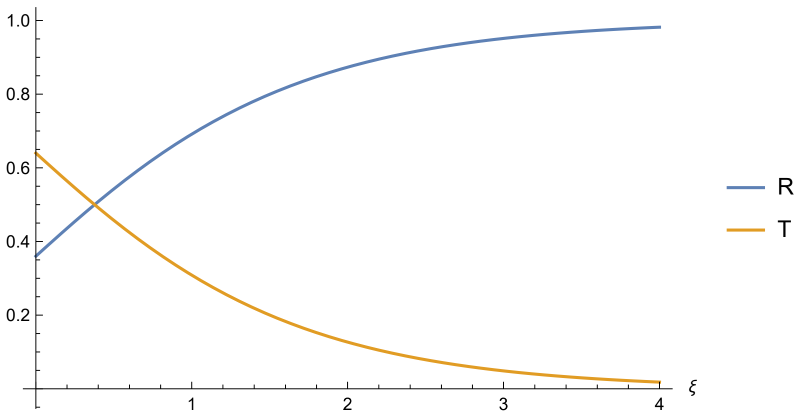
In[∘]:=
$$\left\{R==\frac{\left(1-\frac{e^{-\xi}}{4}\right)^2}{\left(1+\frac{e^{-\xi}}{4}\right)^2},\ T==\frac{e^{-\xi}}{\left(1+\frac{e^{-\xi}}{4}\right)^2}\right\}$$

```
SCMAF[%, SCTaylorSeries, {At[_, 2], ξ}, Head → TildeTilde]
```

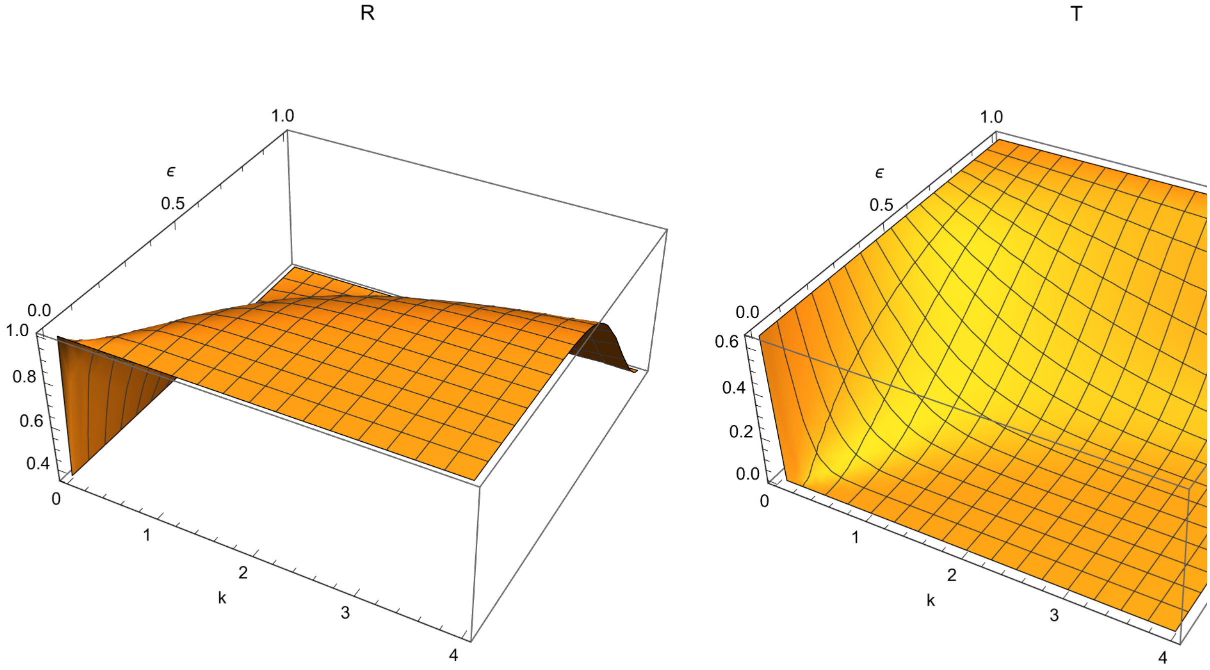
Out[∘]=
$$\left\{R==\frac{\left(1-\frac{e^{-\xi}}{4}\right)^2}{\left(1+\frac{e^{-\xi}}{4}\right)^2},\ T==\frac{e^{-\xi}}{\left(1+\frac{e^{-\xi}}{4}\right)^2}\right\}$$

Out[∘]=
$$\left\{R \approx \frac{9}{25}+\frac{48\,\xi}{125},\ T \approx \frac{16}{25}-\frac{48\,\xi}{125}\right\}$$

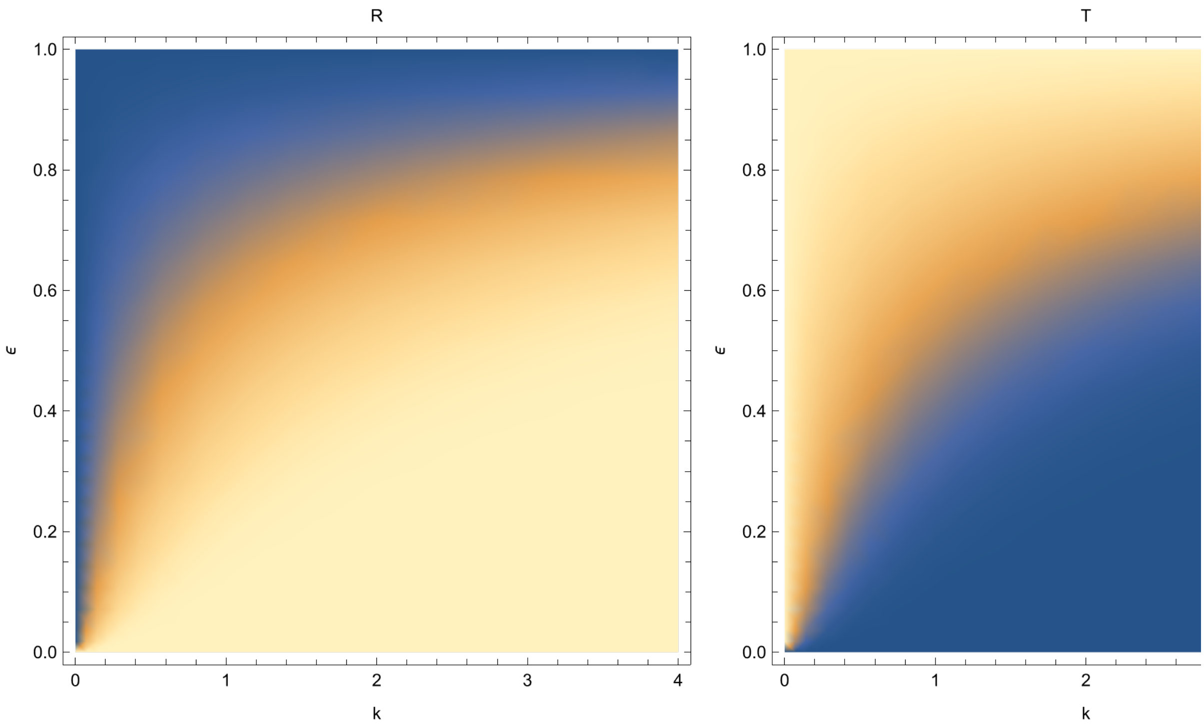
Plot of R and T as functions of $\xi = \frac{8\,k}{3}\left(\sqrt{\frac{1-\epsilon}{\epsilon}} - \sqrt{(1-\epsilon)\,\epsilon}\right)$ ($k = \sqrt{\frac{2\,m\,E}{\hbar^2}}$, $\epsilon = \frac{E}{V_0}$)

Out[∘]=


Plot of R and T as functions of k and ϵ ($k = \sqrt{2\,m\,E/\hbar^2}$, $\epsilon = E/V_0$)


R
T
1.0
ϵ
0.5
0.0
1.0
0.8
0.6
0.4
0
1
2
k
3
4
0.6
0.4
0.2
0.0

Out[∘]=


R
T
1.0
0.8
0.6
ϵ
0.4
0.2
0.0
0
1
2
3
4
k

Integro-differential Equation

Solve the following integro-differential equation.

$$y''(t) = 1 - t\,e^{-t} - \int_0^t z\,y(z)\,dz, \quad y(0) = y_0, \; y'(0) = y'_0. \quad \left({}' \equiv \frac{d}{dt}\right)$$

Ref. M. Rahman, "*Integral Equations and their Applications*," Chapter 6 Integro-differential equations, WIT Press, 2007.

(*a*)

Direct solution using **DSolve** gives a solution, but it is not so convenient.

```
In[ ]:= y''[t] == 1 - t e^-t - Integrate[z y[z], {z, 0, t}]
SCMAF[%, SCDSolve, {All, {y[0] == y0, y'[0] == y'0}, y[t], t}, Hold → {y0, y'0}]
```

(*b*)

Differentiating with respect to *t* and solving the third-order differential equation gives a similar solution.

```
In[ ]:= y''[t] == 1 - t e^-t - ∫_0^t z y[z] dz
SCMAF[%, SCEqMap, {All, D → t},
 SCDSolve, {All, {y[0] == y0, y'[0] == y'0, y''[0] == 1}, y[t], t}, Hold → {y0, y'0}]
```

(*c*)

Applying Laplace transform to both sides of the integro-differential equation, we have

```
In[ ]:= y''[t] == 1 - t e^-t - ∫_0^t z y[z] dz
SCMAF[%, SCEqMap, {All, ℒ, Distribute → True}, SCExpandFunc → {ℒ, t}]
```

Out[ ]= $y''[t] = 1 - e^{-t}\,t - \int_0^t z\,y[z]\,dz$

Out[ ]= $\mathcal{L}[y''[t]] = \mathcal{L}[1] - \mathcal{L}\left[e^{-t}\,t\right] - \mathcal{L}\left[\int_0^t z\,y[z]\,dz\right]$

where $\mathcal{L}$ denotes the Laplace transform operator. The last term $\mathcal{L}\left\{\int_0^t z\,y(z)\,dz\right\}$ can be written as

In[∘]:=
```
SCARA[ℒ[∫_0^t z y[z] ⅆz], ℒ[f_] → ∫_0^∞ ⅇ^(-s t) f ⅆt, Post → SCCombInts,
 SCTransInt, {At[2], Order → {z, t}}, Post → SCSepInts,
 SCEvalInt, {At[2], t, Assumptions → s > 0}, Post → SCFactorInt,
 RA, {At[2], ∫_0^∞ ⅇ^(-s z) z y[z] ⅆz == -ⅆ/ⅆs ∫_0^∞ ⅇ^(-s z) y[z] ⅆz}, RA → ∫_0^∞ ⅇ^(-s z) y[z] ⅆz → ℒ[y[t]]]
```

$$\mathcal{L}\left[\int_0^t z\,y[z]\,dz\right] == \int_0^\infty \int_0^t e^{-s t} z\,y[z]\,dz\,dt$$

$$\mathcal{L}\left[\int_0^t z\,y[z]\,dz\right] == \frac{1}{s}\int_0^\infty e^{-s z} z\,y[z]\,dz$$

Out[∘]= $$\mathcal{L}\left[\int_0^t z\,y[z]\,dz\right] == -\frac{1}{s}\,\frac{d\mathcal{L}[y[t]]}{ds}$$

In general, for $n \geq 0$,

In[∘]:=
```
SCARA[ℒ[∫_0^t z^n y[z] ⅆz], ℒ[f_] → ∫_0^∞ ⅇ^(-s t) f ⅆt, Post → SCCombInts,
 SCTransInt, {At[2], Order → {z, t}}, Post → SCSepInts,
 SCEvalInt, {At[2], t, Assumptions → s > 0}, Post → SCFactorInt,
 RA, {At[2], ∫_0^∞ ⅇ^(-s z) z^n y[z] ⅆz == (-1)^n ⅆ^n/ⅆs^n ∫_0^∞ ⅇ^(-s z) y[z] ⅆz}, RA → ∫_0^∞ ⅇ^(-s z) y[z] ⅆz → ℒ[y[t]]]
```

$$\mathcal{L}\left[\int_0^t z^n\,y[z]\,dz\right] == \int_0^\infty \int_0^t e^{-s t} z^n\,y[z]\,dz\,dt$$

$$\mathcal{L}\left[\int_0^t z^n\,y[z]\,dz\right] == \frac{1}{s}\int_0^\infty e^{-s z} z^n\,y[z]\,dz$$

Out[∘]= $$\mathcal{L}\left[\int_0^t z^n\,y[z]\,dz\right] == \frac{(-1)^n}{s}\,\frac{d^n\mathcal{L}[y[t]]}{ds^n}$$

Hence, we have

In[3]:=
```
ℒ[y''[t]] == ℒ[1] - ℒ[ⅇ^-t t] - ℒ[∫_0^t z y[z] ⅆz]
SCMAF[%, RA, {All, ℒ[∫_0^t z y[z] ⅆz] == -1/s ⅆℒ[y[t]]/ⅆs}, ,
 RA, {All, ℒ[f_] :→ LaplaceTransform[f, t, s]}, Hold → ℒ[y[t]],
 RA → {LaplaceTransform[y[t], t, s] == ℒ[y[t]], y[0] == y0, y'[0] == y'0},
 SCSolve, {All, ⅆℒ[y[t]]/ⅆs, Post → Collect → {ℒ[y[t]], Simplify}}, ,
 SCDSolve, {All, ℒ[y[t]], s, Post → Expand}, Post → PowerExpand,
 Collect, {ⅇ^(s^4/4) c1 + _, {-1 + y0, 1 + y'0}, Simplify},
 ReplVar → {-1 + y0, 1 + y'0}, ChangeSign → -1 + Erf[s^2/2]]
```

Out[3]= $$\mathcal{L}[y''[t]] == \mathcal{L}[1] - \mathcal{L}\left[e^{-t}\,t\right] - \mathcal{L}\left[\int_0^t z\,y[z]\,dz\right]$$

$$\mathcal{L}[y''[t]] == \frac{1}{s}\,\frac{d\mathcal{L}[y[t]]}{ds} + \mathcal{L}[1] - \mathcal{L}\left[e^{-t}\,t\right]$$

$$\frac{d\mathcal{L}[y[t]]}{ds} == s^3\,\mathcal{L}[y[t]] - s\left(\frac{1}{s} - \frac{1}{(1+s)^2} + s\,y_0 + y_0'\right)$$

$$\mathcal{L}[y[t]] == \frac{1}{2}\,e^{\frac{s^4}{4}}\sqrt{\pi} + \frac{1}{1+s} + e^{\frac{s^4}{4}}\,c_1 - \frac{1}{2}\,e^{\frac{s^4}{4}}\sqrt{\pi}\,\mathrm{Erf}\left[\frac{s^2}{2}\right] - \frac{e^{\frac{s^4}{4}}}{\sqrt{2}}\,\Gamma\left[\frac{3}{4},\frac{s^4}{4}\right] + \frac{e^{\frac{s^4}{4}}\,y_0}{\sqrt{2}}\,\Gamma\left[\frac{3}{4},\frac{s^4}{4}\right] + \frac{1}{2}\,e^{\frac{s^4}{4}}\sqrt{\pi}\,y_0' - \frac{1}{2}\,e^{\frac{s^4}{4}}\sqrt{\pi}\,y_0'\,\mathrm{Erf}\left[\frac{s^2}{2}\right]$$

Out[4]= $$\mathcal{L}[y[t]] == \frac{1}{1+s} + e^{\frac{s^4}{4}}\,c_1 + \frac{e^{\frac{s^4}{4}}\,(-1+y_0)}{\sqrt{2}}\,\Gamma\left[\frac{3}{4},\frac{s^4}{4}\right] + \frac{1}{2}\,e^{\frac{s^4}{4}}\sqrt{\pi}\,(1+y_0')\times\left(1-\mathrm{Erf}\left[\frac{s^2}{2}\right]\right)$$

The inverse transform gives

In[ ]:=
```
y[t] == ℒ^-1[1/(1 + s) + e^(s^4/4) c1 + (e^(s^4/4) (-1 + y0))/Sqrt[2] Γ[3/4, s^4/4] + 1/2 e^(s^4/4) Sqrt[π] (1 + y0′) × (1 - Erf[s^2/2])]
SCMAF[%, SCExpandFunc, {At[2], ℒ^-1, s},
  RA, {At[2], ℒ^-1[1/(1 + s)] → InverseLaplaceTransform[1/(1 + s), s, t]}]
```

Out[ ]= $$y[t] == \mathcal{L}^{-1}\left[\frac{1}{1+s} + e^{\frac{s^4}{4}}\,c_1 + \frac{e^{\frac{s^4}{4}}\,(-1+y_0)}{\sqrt{2}}\,\Gamma\left[\frac{3}{4},\frac{s^4}{4}\right] + \frac{1}{2}\,e^{\frac{s^4}{4}}\sqrt{\pi}\,(1+y_0')\times\left(1-\mathrm{Erf}\left[\frac{s^2}{2}\right]\right)\right]$$

$$y[t] == c_1\,\mathcal{L}^{-1}\left[e^{\frac{s^4}{4}}\right] + \mathcal{L}^{-1}\left[\frac{1}{1+s}\right] + \frac{1}{2}\sqrt{\pi}\,(1+y_0')\,\mathcal{L}^{-1}\left[e^{\frac{s^4}{4}}\left(1-\mathrm{Erf}\left[\frac{s^2}{2}\right]\right)\right] + \frac{-1+y_0}{\sqrt{2}}\,\mathcal{L}^{-1}\left[e^{\frac{s^4}{4}}\,\Gamma\left[\frac{3}{4},\frac{s^4}{4}\right]\right]$$

Out[ ]= $$y[t] == e^{-t} + c_1\,\mathcal{L}^{-1}\left[e^{\frac{s^4}{4}}\right] + \frac{1}{2}\sqrt{\pi}\,(1+y_0')\,\mathcal{L}^{-1}\left[e^{\frac{s^4}{4}}\left(1-\mathrm{Erf}\left[\frac{s^2}{2}\right]\right)\right] + \frac{-1+y_0}{\sqrt{2}}\,\mathcal{L}^{-1}\left[e^{\frac{s^4}{4}}\,\Gamma\left[\frac{3}{4},\frac{s^4}{4}\right]\right]$$

where the constant c_1 is determined to satisfy $y(0) = y_0$.

(*d*)

Direct solution using **`SCIntSolve`**

In[ ]:=
```
y''[t] == 1 - t e^-t - ∫_0^t z y[z] dz
SCMAF[%, SCIntSolve, {All, y[t], t, Inverse → Inactive, ReplVar → s},
  Post → PowerExpand, RA → {y[0] == y0, y'[0] == y'0},
  Collect, {e^(s^4/4) c1 + _, {-1 + y0, 1 + y'0}, Simplify},
  ReplVar → {-1 + y0, 1 + y'0}, ChangeSign → -1 + Erf[s^2/2],
  SCExpandFunc, {At[2], InverseLaplaceTransform, {s, t}},
  HoldVar → {-1 + y0, 1 + y'0, 1 - Erf[s^2/2]},
  Post → {Inactivate → InverseLaplaceTransform, Activate}]
```

Out[ ]= $y''[t] == 1 - e^{-t} t - \int_0^t z\, y[z]\, dz$

$y[t] == \text{InverseLaplaceTransform}\left[\frac{1}{1+s} + e^{\frac{s^4}{4}} c_1 + \frac{e^{\frac{s^4}{4}} (-1 + y_0)}{\sqrt{2}} \Gamma\left[\frac{3}{4}, \frac{s^4}{4}\right] + \frac{1}{2} e^{\frac{s^4}{4}} \sqrt{\pi}\, (1 + y'_0) \times \left(1 - \text{Erf}\left[\frac{s^2}{2}\right]\right), s, t\right]$

Out[ ]= $y[t] == e^{-t} + c_1 \text{InverseLaplaceTransform}\left[e^{\frac{s^4}{4}}, s, t\right] + \frac{1}{2} \sqrt{\pi}\, (1 + y'_0) \text{InverseLaplaceTransform}\left[e^{\frac{s^4}{4}} \left(1 - \text{Erf}\left[\frac{s^2}{2}\right]\right), s, t\right] + \frac{-1 + y_0}{\sqrt{2}} \text{InverseLaplaceTransform}\left[e^{\frac{s^4}{4}} \Gamma\left[\frac{3}{4}, \frac{s^4}{4}\right], s, t\right]$

(*e*)

It is possible to obtain the solution using power series. Substitute $y(t)$ with the series

$$y(t) = \sum_{n=0}^{\infty} a_n t^n,$$

and it can be shown

In[∘]:=
```
y''[t] == 1 - t e^-t - ∫_0^t z y[z] dz
SCMAF[%, SCFuncRA, {All, y[t_] → Sum[a_n t^n, {n, 0, ∞}]},
  SCIntInSum, At[2], Post → SCFactorInt,
  SCEvalInt, {At[2], Indefinite → True}, RA → 0^(2+n) → 0,
  SCPowerSeries, {e^-t, n}, Post → {At[2], {SCInSum, PowerExpand}},
  SCSumShiftVar, {Sum[t^(n+s_) f_, {n, 0, ∞}], {n, -s}},
  SCSumChangeLimits, {All, {n, 2, ∞}}, Post → SCEqMerge,
  SCMergeSums, {At[1], Post → SCFactor → t^n (1 + n) × (2 + n)},
  SCFactorialShift, {(-1 + n)!, 1},
  SCDenomApply, {At[1], SCSimpFactorial}, Collect → t]
```

Out[∘]= $y''[t] == 1 - e^{-t} t - \int_0^t z\, y[z]\, dz$

$-1 + t + \sum_{n=2}^{\infty} (1+n) \times (2+n)\, t^n \left(\frac{(-1)^{1+n} n}{(1+n) \times (2+n)\, n!} + \frac{a_{-2+n}}{n\,(1+n) \times (2+n)} + a_{2+n} \right) + 2 a_2 + 6 t a_3 == 0$

Out[∘]= $-1 + \sum_{n=2}^{\infty} (1+n) \times (2+n)\, t^n \left(\frac{(-1)^{1+n} n}{(2+n)!} + \frac{a_{-2+n}}{n\,(1+n) \times (2+n)} + a_{2+n} \right) + 2 a_2 + t\,(1 + 6 a_3) == 0$

Since

In[∘]:=
```
y[t] == Sum[a_n t^n, {n, 0, ∞}]
SCMAF[%, SCEqMap, {All, D → t},
  SCSumShiftVar, {At[2], {n, 1}}, SCSumChangeLimits → {{n, 0, ∞}}]
```

Out[∘]= $y[t] == \sum_{n=0}^{\infty} t^n a_n$

$y'[t] == \sum_{n=0}^{\infty} n\, t^{-1+n} a_n$

Out[∘]= $y'[t] == \sum_{n=0}^{\infty} (1+n)\, t^n a_{1+n}$

and thus,

In[ ]:=

$$\left\{y[t] == \sum_{n=0}^{\infty} a_n\, t^n,\; y'[t] == \sum_{n=0}^{\infty} (1+n)\, t^n\, a_{1+n}\right\}$$

```
SCMAF[%, RA, {All, t == 0}, RA → {0^n == δ_n, y[0] == y_0, y'[0] == y'_0},
 SCEvalSumDelta, All]
```

Out[ ]=

$$\left\{y[t] == \sum_{n=0}^{\infty} t^n\, a_n,\; y'[t] == \sum_{n=0}^{\infty} (1+n)\, t^n\, a_{1+n}\right\}$$

$$\left\{y_0 == \sum_{n=0}^{\infty} a_n\, \delta_n,\; y'_0 == \sum_{n=0}^{\infty} (1+n)\, a_{1+n}\, \delta_n\right\}$$

Out[ ]= $\{y_0 == a_0,\; y'_0 == a_1\}$

we have

$$a_0 = y_0, \quad a_1 = y'_0, \quad a_2 = \frac{1}{2}, \quad a_3 = -\frac{1}{6}, \quad a_{n+2} = \frac{(-1)^n\, n}{(n+2)!} - \frac{a_{n-2}}{n\,(n+1)\,(n+2)}, \quad n \geq 2.$$

Try to solve the recursion relation using **RSolve**.

$$\text{SCRSolve}\left[a_{n+2} == \frac{(-1)^n\, n}{(n+2)!} - \frac{a_{n-2}}{n\,(n+1)\,(n+2)},\; \left\{a_0 == y_0,\, a_1 == y'_0,\, a_2 == \frac{1}{2},\, a_3 == -\frac{1}{6}\right\},\, a_n,\, n\right]$$

Out[ ]=

$$a_n == \frac{(-1)^{\frac{7}{4}+\frac{n}{4}}\, \pi \left(\frac{i}{2}\right)^n}{e^{1/4}\,(-1+n)\times(1+n)\,\Gamma\left[-\frac{1}{4}+\frac{n}{4}\right]\times\Gamma\left[1+\frac{n}{2}\right]} + \frac{(-1)^{\frac{7}{4}+\frac{5n}{4}}\,(2\,i)^{-n}\,\pi}{e^{1/4}\,(-1+n)\times(1+n)\,\Gamma\left[-\frac{1}{4}+\frac{n}{4}\right]\times\Gamma\left[1+\frac{n}{2}\right]} +$$

$$\frac{5\,\langle\!\langle 1 \rangle\!\rangle\,\pi\,\langle\!\langle 1 \rangle\!\rangle^n}{\langle\!\langle 1 \rangle\!\rangle\,\langle\!\langle 1 \rangle\!\rangle} + \langle\!\langle 331 \rangle\!\rangle + \frac{\langle\!\langle 1 \rangle\!\rangle}{\langle\!\langle 1 \rangle\!\rangle} + \frac{\left(\frac{1}{105}+\frac{i}{105}\right)(-1)^{\langle\!\langle 1 \rangle\!\rangle}\, 2^{\langle\!\langle 1 \rangle\!\rangle}\left(\langle\!\langle 63 \rangle\!\rangle + \langle\!\langle 1 \rangle\!\rangle\right)}{e^{1/4}\sqrt{\pi}\,\Gamma\left[\frac{1}{4}\right]\times\Gamma\left[\frac{3}{4}\right]\times\Gamma\left[\frac{9}{4}\right]\times\Gamma\left[\frac{11}{4}\right]\times\Gamma\left[\frac{3}{4}+\frac{n}{4}\right]\times\Gamma\left[1+\frac{n}{2}\right]} +$$

$$\frac{\left(\frac{1}{105}+\frac{i}{105}\right)(-1)^{n/4}\, 2^{-7-n}\,\text{Sin}\left[\frac{n\pi}{2}\right]\left(\langle\!\langle 27 \rangle\!\rangle + \langle\!\langle 1 \rangle\!\rangle - 3360\, i\, e^{1/4}\sqrt{2\pi}\,\Gamma\left[\frac{1}{4}\right]\times\Gamma\left[\frac{3}{4}\right]\times\Gamma\left[\frac{9}{4}\right]\times\Gamma\left[\frac{11}{4}\right]\, y'[0]\right)}{e^{1/4}\,\Gamma\left[\frac{1}{4}\right]\times\Gamma\left[\frac{3}{4}\right]\times\Gamma\left[\frac{9}{4}\right]\times\Gamma\left[\frac{11}{4}\right]\times\Gamma\left[\frac{3}{4}+\frac{n}{4}\right]\times\Gamma\left[1+\frac{n}{2}\right]}$$

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From the first several terms

In[ ]:=

$$\text{Module}\left[\{N = 11,\, \text{tbl}\},\; \text{tbl} = \text{Expand}\left[\text{RecurrenceTable}\left[\left\{a_{n+2} == \frac{(-1)^n\, n}{(n+2)!} - \frac{a_{n-2}}{n\,(n+1)\,(n+2)},\, a_0 == y_0,\, a_1 == y'_0,\, a_2 == \frac{1}{2},\, a_3 == -\frac{1}{6}\right\},\, a_n,\, \{n, 0, N\}\right]\right];\right.$$

```
Thread[Table[a_n, {n, 0, N}] == (If[NumberQ[#], SCFactorInteger[#, ℤ], #] & /@ tbl)]]
```

Out[ ]=

$$\left\{a_0 == y_0,\, a_1 == y'_0,\, a_2 == \frac{1}{2},\, a_3 == (-1)\cdot\frac{1}{3}\cdot\frac{1}{2},\, a_4 == \frac{1}{12} - \frac{y_0}{24},\, a_5 == -\frac{1}{40} - \frac{y'_0}{60},\, a_6 == \frac{1}{6}\cdot\frac{1}{5}\cdot\frac{1}{4}\cdot\frac{1}{3}\cdot\frac{1}{2},\right.$$

$$a_7 == (-1)\cdot\frac{1}{7}\cdot\frac{1}{6}\cdot\frac{1}{5}\cdot\frac{1}{4}\cdot\frac{1}{3}\cdot\frac{1}{2},\, a_8 == -\frac{1}{10080} + \frac{y_0}{8064},\, a_9 == \frac{11}{362880} + \frac{y'_0}{30240},$$

$$\left. a_{10} == \frac{1}{10}\cdot\frac{1}{9}\cdot\frac{1}{8}\cdot\frac{1}{7}\cdot\frac{1}{6}\cdot\frac{1}{5}\cdot\frac{1}{4}\cdot\frac{1}{3}\cdot\frac{1}{2},\, a_{11} == (-1)\cdot\frac{1}{11}\cdot\frac{1}{10}\cdot\frac{1}{9}\cdot\frac{1}{8}\cdot\frac{1}{7}\cdot\frac{1}{6}\cdot\frac{1}{5}\cdot\frac{1}{4}\cdot\frac{1}{3}\cdot\frac{1}{2}\right\}$$

we put

$$a_n = \frac{(-1)^n}{n!} + b_n,$$

where b_n is a sequence that depends on y_0 and y_0'. The recursion relation for b_n is

In[ ]:=
```
a_{n+2} == (-1)^n n/(n+2)! - a_{n-2}/(n (n+1) (n+2))
SCMAF[%, RA, {All, a_{n_} -> (-1)^n/n! + b_n}, Post -> {Expand, SCEqMerge},
  SCFactorialShift, {(-2 + n)!, 1},
  SCDenomApply, {At[1], SCSimpFactorial},
  SCEqSep, {All, b}, Hold -> n + _,
  Simplify, At[2], AddComment -> "n ≥ 2."]
```

Out[ ]= $a_{2+n} == \frac{(-1)^n n}{(2+n)!} - \frac{a_{-2+n}}{n(1+n)\times(2+n)}$

$\frac{b_{-2+n}}{n(1+n)\times(2+n)} + b_{2+n} == \frac{(-1)^{1+n}}{(2+n)!} + \frac{(-1)^{1+n}(-1+n)}{(2+n)!} + \frac{(-1)^n n}{(2+n)!}$

$\frac{b_{-2+n}}{n(1+n)\times(2+n)} + b_{2+n} == 0$

n ≥ 2.

The initial conditions for b_n are

In[ ]:=
```
{a_0 == y_0, a_1 == y'_0, a_2 == 1/2, a_3 == -1/6}
SCMAF[%, RA, {All, a_{n_} -> (-1)^n/n! + b_n}, SCSolve -> {{b_0, b_1, b_2, b_3}}]
```

Out[ ]= $\{a_0 == y_0,\ a_1 == y_0',\ a_2 == \frac{1}{2},\ a_3 == -\frac{1}{6}\}$

Out[ ]= $\{b_0 == -1 + y_0,\ b_1 == 1 + y_0',\ b_2 == 0,\ b_3 == 0\}$

The solution for b_n

In[∘]:=
```
b_{-2+n}/(n (1 + n) × (2 + n)) + b_{2+n} == 0
SCMAF[%, SCRSolve, {All, {b_0 == -1 + y_0, b_1 == 1 + y'_0, b_2 == 0, b_3 == 0}, b_n, n},
 SCSubdiv, {All, 4, n}, SCExpandArg → Gamma | Cos | Sin,
 Simplify, {At[_, 2], n ∈ ℤ}]
```

Out[∘]= $\frac{b_{-2+n}}{n\,(1+n)\times(2+n)}+b_{2+n}==0$

$$\Big\{b_{4n}==\frac{1}{\Gamma[1+2n]\times\Gamma\left[\frac{3}{4}+n\right]}(-1)^{n}\,2^{-2-4n}\Big(-(-1)^{3/4}\sqrt{\pi}+(-1)^{\frac{3}{4}+4n}\sqrt{\pi}-2\,\Gamma\left[\frac{3}{4}\right]-2\,\mathrm{Cos}[2n\pi]\,\Gamma\left[\frac{3}{4}\right]-2\,(-1)^{3/4}\sqrt{\pi}\,\mathrm{Sin}[2n\pi]+2\,y_0\,\Gamma\left[\frac{3}{4}\right]+2\,\mathrm{Cos}[2n\pi]\,y_0\,\Gamma\left[\frac{3}{4}\right]-(-1)^{3/4}\sqrt{\pi}\,y'_0+(-1)^{\frac{3}{4}+4n}\sqrt{\pi}\,y'_0-2\,(-1)^{3/4}\sqrt{\pi}\,\mathrm{Sin}[2n\pi]\,y'_0\Big),$$

$$b_{1+4n}==\frac{1}{\Gamma[1+n]\times\Gamma\left[\frac{3}{2}+2n\right]}(-1)^{\frac{1}{4}\times(1+4n)}\,2^{-3-4n}\Big(-(-1)^{3/4}\sqrt{\pi}+(-1)^{\frac{7}{4}+4n}\sqrt{\pi}-2\,(-1)^{3/4}\sqrt{\pi}\,\mathrm{Cos}[2n\pi]+2\,\mathrm{Sin}[2n\pi]\,\Gamma\left[\frac{3}{4}\right]-2\,\mathrm{Sin}[2n\pi]\,y_0\,\Gamma\left[\frac{3}{4}\right]-(-1)^{3/4}\sqrt{\pi}\,y'_0+(-1)^{\frac{7}{4}+4n}\sqrt{\pi}\,y'_0-2\,(-1)^{3/4}\sqrt{\pi}\,\mathrm{Cos}[2n\pi]\,y'_0\Big),$$

$$b_{2+4n}==\frac{1}{\Gamma[2+2n]\times\Gamma\left[\frac{5}{4}+n\right]}(-1)^{\frac{1}{4}\times(2+4n)}\,2^{-4-4n}\Big(-(-1)^{3/4}\sqrt{\pi}+(-1)^{\frac{11}{4}+4n}\sqrt{\pi}-2\,\Gamma\left[\frac{3}{4}\right]+2\,\mathrm{Cos}[2n\pi]\,\Gamma\left[\frac{3}{4}\right]+2\,(-1)^{3/4}\sqrt{\pi}\,\mathrm{Sin}[2n\pi]+2\,y_0\,\Gamma\left[\frac{3}{4}\right]-2\,\mathrm{Cos}[2n\pi]\,y_0\,\Gamma\left[\frac{3}{4}\right]-(-1)^{3/4}\sqrt{\pi}\,y'_0+(-1)^{\frac{11}{4}+4n}\sqrt{\pi}\,y'_0+2\,(-1)^{3/4}\sqrt{\pi}\,\mathrm{Sin}[2n\pi]\,y'_0\Big),\ b_{3+4n}==\frac{1}{\Gamma\left[\frac{3}{2}+n\right]\times\Gamma\left[\frac{5}{2}+2n\right]}(-1)^{\frac{1}{4}\times(3+4n)}\,2^{-5-4n}\Big(-(-1)^{3/4}\sqrt{\pi}+(-1)^{\frac{15}{4}+4n}\sqrt{\pi}+2\,(-1)^{3/4}\sqrt{\pi}\,\mathrm{Cos}[2n\pi]-2\,\mathrm{Sin}[2n\pi]\,\Gamma\left[\frac{3}{4}\right]+2\,\mathrm{Sin}[2n\pi]\,y_0\,\Gamma\left[\frac{3}{4}\right]-(-1)^{3/4}\sqrt{\pi}\,y'_0+(-1)^{\frac{15}{4}+4n}\sqrt{\pi}\,y'_0+2\,(-1)^{3/4}\sqrt{\pi}\,\mathrm{Cos}[2n\pi]\,y'_0\Big)\Big\}$$

Out[∘]= $\left\{b_{4n}==\frac{\left(-\frac{1}{16}\right)^{n}(-1+y_0)\,\Gamma\left[\frac{3}{4}\right]}{\Gamma[1+2n]\times\Gamma\left[\frac{3}{4}+n\right]},\ b_{1+4n}==\frac{(-1)^{n}\,2^{-1-4n}\sqrt{\pi}\,(1+y'_0)}{\Gamma[1+n]\times\Gamma\left[\frac{3}{2}+2n\right]},\ b_{2+4n}==0,\ b_{3+4n}==0\right\}$

Therfore, the solution $y(t)$ of the integro-differential equation is

In[•]:=

```
y[t] == Sum[a_n t^n, {n, 0, ∞}]
SCMAF[%, RA, {At[2], a_n == (-1)^n/n! + b_n}, Post → SCExpandSumAll,
  SCEvalSum, Sum[(-1)^n t^n/n!, {n, 0, ∞}],
  SCSumSubdiv, {At[2], 4},
  RA → {b_{4 n} == (-1/16)^n (-1 + y_0) Γ[3/4]/(Γ[1 + 2 n] × Γ[3/4 + n]), b_{1+4 n} == (-1)^n 2^(-1-4 n) Sqrt[π] (1 + y'_0)/(Γ[1 + n] × Γ[3/2 + 2 n]), b_{2+4 n} == 0, b_{3+4 n} == 0},
  Post → {Simplify, SCFactorSum},
  SCEvalSum, At[2], Post → SCFuncShort]
```

Out[•]= $y[t] == \sum_{n=0}^{\infty} t^n a_n$

$$y[t] == e^{-t} + (-1 + y_0)\, \Gamma\left[\frac{3}{4}\right] \sum_{n=0}^{\infty} \frac{\left(-\frac{1}{16}\right)^n t^{4n}}{\Gamma[1 + 2n] \times \Gamma\left[\frac{3}{4} + n\right]} + \frac{1}{2} \sqrt{\pi}\, t\, (1 + y'_0) \sum_{n=0}^{\infty} \frac{\left(-\frac{1}{16}\right)^n t^{4n}}{\Gamma[1 + n] \times \Gamma\left[\frac{3}{2} + 2n\right]}$$

Out[•]= $y[t] == e^{-t} + (-1 + y_0)\, {}_0F_2\left[\{\}, \left\{\frac{1}{2}, \frac{3}{4}\right\}, -\frac{t^4}{64}\right] + t\, (1 + y'_0)\, {}_0F_2\left[\{\}, \left\{\frac{3}{4}, \frac{5}{4}\right\}, -\frac{t^4}{64}\right]$

The asymptotic solution in the limit $t \to +\infty$:

In[•]:=

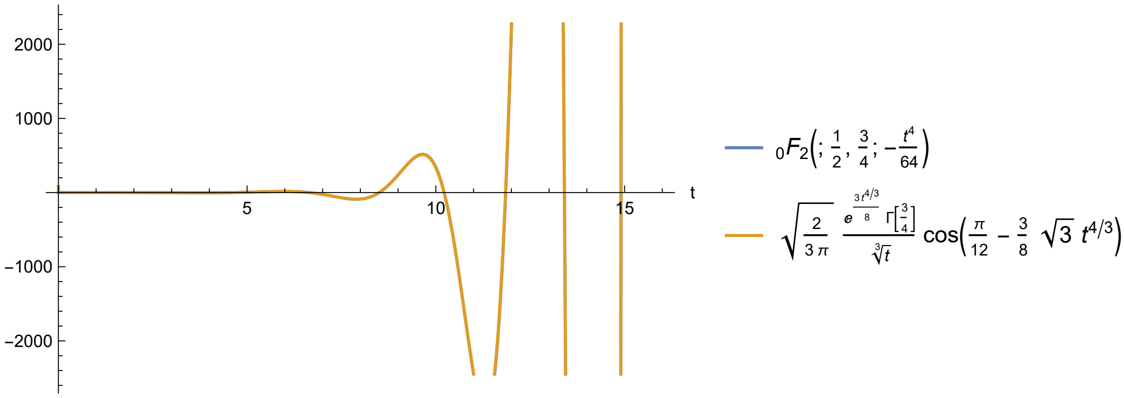
```
y[t] == e^-t + (-1 + y_0) 0F2[{}, {1/2, 3/4}, -t^4/64] + t (1 + y'_0) 0F2[{}, {3/4, 5/4}, -t^4/64]
SCMAF[%, SCFuncNormal, At[2],
  Asymptotic, {_HypergeometricPFQ, t → ∞}, Head → Tilde,
  PowerExpand, At[2], Post → {SCComplexToExp, (-1)^p_},
  2 Re[#] &, {{-e^(11 i π/12 + 3/4 e^(i π/3) t^(4/3))}, {-e^(2 i π/3 + 3/4 e^(i π/3) t^(4/3))}}, Post → {PowerExpand, SCComplexExpand},
  SCFactor, {Sqrt[2/(3 π)] e^(3 t^(4/3)/8) (-1 + y_0) Γ[3/4]/t^(1/3) Cos[π/12 - 3/8 Sqrt[3] t^(4/3)] +
    Sqrt[2/3] e^(3 t^(4/3)/8) (1 + y'_0)/t^(1/3) Sin[π/6 + 3/8 Sqrt[3] t^(4/3)], Sqrt[2/3] e^(3 t^(4/3)/8)/t^(1/3)}]
```

Out[•]= $y[t] == e^{-t} + (-1 + y_0)\, {}_0F_2\left[\{\}, \left\{\frac{1}{2}, \frac{3}{4}\right\}, -\frac{t^4}{64}\right] + t\, (1 + y'_0)\, {}_0F_2\left[\{\}, \left\{\frac{3}{4}, \frac{5}{4}\right\}, -\frac{t^4}{64}\right]$

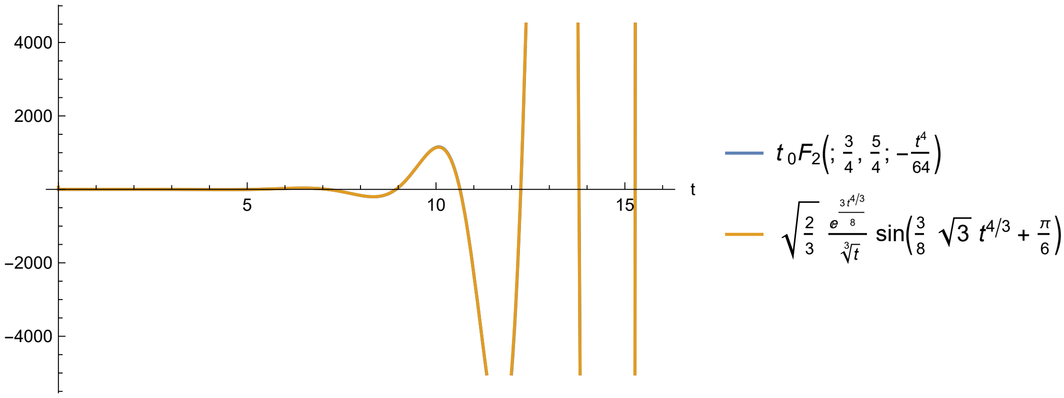
$$y[t] \sim e^{-t} + \sqrt{\frac{2}{3\pi}} \frac{e^{\frac{3 t^{4/3}}{8}} (-1 + y_0)\, \Gamma\left[\frac{3}{4}\right]}{t^{1/3}} \operatorname{Cos}\left[\frac{\pi}{12} - \frac{3}{8}\sqrt{3}\, t^{4/3}\right] + \sqrt{\frac{2}{3}} \frac{e^{\frac{3 t^{4/3}}{8}} (1 + y'_0)}{t^{1/3}} \operatorname{Sin}\left[\frac{\pi}{6} + \frac{3}{8}\sqrt{3}\, t^{4/3}\right]$$

Out[•]= $y[t] \sim e^{-t} + \sqrt{\frac{2}{3}} \frac{e^{\frac{3 t^{4/3}}{8}}}{t^{1/3}} \left(\frac{(-1 + y_0)\, \Gamma\left[\frac{3}{4}\right]}{\sqrt{\pi}} \operatorname{Cos}\left[\frac{\pi}{12} - \frac{3}{8}\sqrt{3}\, t^{4/3}\right] + (1 + y'_0) \operatorname{Sin}\left[\frac{\pi}{6} + \frac{3}{8}\sqrt{3}\, t^{4/3}\right]\right)$

Graphic visualization of the asymptotic forms of ${}_0F_2\left(; \frac{1}{2}, \frac{3}{4}; -\frac{t^4}{64}\right)$ and $t\, {}_0F_2\left(; \frac{3}{4}, \frac{5}{4}; -\frac{t^4}{64}\right)$



Out[ ]=



Verify the solution by back substitution in the integro-differential equation and the initial conditions.

In[ ]:=

$$\left\{y''[t] == 1 - t\, e^{-t} - \int_0^t z\, y[z]\, dz,\ y[0] == y_0,\ y'[0] == y'_0\right\}$$

$$\text{SCMAF}\Big[\%, \text{SCFuncRA}, \Big\{\text{All}, y[t\_] \to e^{-t} + (-1 + y_0)\ \text{HypergeometricPFQ}\Big[\{\}, \Big\{\frac{1}{2}, \frac{3}{4}\Big\}, -\frac{t^4}{64}\Big] + t\,(1 + y'_0)\ \text{HypergeometricPFQ}\Big[\{\}, \Big\{\frac{3}{4}, \frac{5}{4}\Big\}, -\frac{t^4}{64}\Big]\Big\},$$

$$\text{SCEvalInt}, \text{At}[1], \text{FullSimplify}, \text{At}[1]\Big]$$

Out[ ]=

$$\left\{y''[t] == 1 - e^{-t}\, t - \int_0^t z\, y[z]\, dz,\ y[0] == y_0,\ y'[0] == y'_0\right\}$$

$$\Big\{e^{-t} - \frac{1}{2} t^2 (-1 + y_0)\ \text{HypergeometricPFQ}\Big[\{\}, \Big\{\frac{3}{2}, \frac{7}{4}\Big\}, -\frac{t^4}{64}\Big] + \frac{1}{252} t^6 (-1 + y_0)\ \text{HypergeometricPFQ}\Big[\{\}, \Big\{\frac{5}{2}, \frac{11}{4}\Big\}, -\frac{t^4}{64}\Big] - \frac{2}{15} t^3 (1 + y'_0)\ \text{HypergeometricPFQ}\Big[\{\}, \Big\{\frac{7}{4}, \frac{9}{4}\Big\}, -\frac{t^4}{64}\Big] + t\,(1 + y'_0)\Big(-\frac{t^2}{5}\ \text{HypergeometricPFQ}\Big[\{\}, \Big\{\frac{7}{4}, \frac{9}{4}\Big\}, -\frac{t^4}{64}\Big] + \frac{t^6}{945}\ \text{HypergeometricPFQ}\Big[\{\}, \Big\{\frac{11}{4}, \frac{13}{4}\Big\}, -\frac{t^4}{64}\Big]\Big) ==$$

$$1 - e^{-t}\left(-1 + e^{t} - t\right) - e^{-t}\, t - \frac{1}{2} t^2 (-1 + y_0)\ \text{HypergeometricPFQ}\Big[\{\}, \Big\{\frac{3}{4}, \frac{3}{2}\Big\}, -\frac{t^4}{64}\Big] - \frac{1}{3} t^3 (1 + y'_0)\ \text{HypergeometricPFQ}\Big[\{\}, \Big\{\frac{5}{4}, \frac{7}{4}\Big\}, -\frac{t^4}{64}\Big], \text{True}, \text{True}\Big\}$$

Out[ ]= {True, True, True}

Thank You for the Attention.