Nov. 22 2006

Lecture 22: Differential Operators, Harmonic Oscillators

Reading:
Kreyszig Sections: 2.3,2.4, 2.7 (pages59–60, 61–69, 78–83)

Differential Operators

The idea of a function as "something" that takes a value (real, complex, vector, etc.) as "input" and returns "something else" as "output" should be very familiar and useful.

This idea can be generalized to *operators* that take a function as an argument and return another function.

The derivative operator operates on a function and returns another function that describes how the function changes:

$$\begin{aligned}\mathcal{D}[f(x)] &= \frac{df}{dx}\\ \mathcal{D}[\mathcal{D}[f(x)]] = \mathcal{D}^2[f(x)] &= \frac{d^2f}{dx^2}\\ \mathcal{D}^n[f(x)] &= \frac{d^nf}{dx^n}\\ \mathcal{D}[\alpha f(x)] &= \alpha D[f(x)]\\ \mathcal{D}[f(x)+g(x)] &= D[f(x)] + D[g(x)]\end{aligned} \tag{22-1}$$

The last two equations above indicate that the "differential operator" is a linear operator.

The integration operator is the right-inverse of $\mathcal{D}$

$$\mathcal{D}[\mathcal{I}[f(x)]] = \mathcal{D}[\int f(x)dx] \tag{22-2}$$

but is only the left-inverse up to an arbitrary constant.

Consider the differential operator that returns a constant multiplied by itself

$$\mathcal{D}f(x) = \lambda f(x) \tag{22-3}$$

which is another way to write the the homogenous linear first-order ODE and has the same form as an eigenvalue equation. In fact, $f(x) = \exp(\lambda x)$, can be considered an *eigenfunction* of Eq. 22-3.

For the homogeneous second-order equation,

$$\left(\mathcal{D}^2 + \beta\mathcal{D} - \gamma\right)[f(x)] = 0 \tag{22-4}$$

It was determined that there were two eigensolutions that can be used to span the entire solution space:

$$f(x) = C_+e^{\lambda_+ x} + C_-e^{\lambda_- x} \tag{22-5}$$

Operators can be used algebraically, consider the inhomogeneous second-order ODE

$$\left(a\mathcal{D}^2 + b\mathcal{D} + c\right)[y(x)] = x^3 \tag{22-6}$$

By treating the operator as an algebraic quantity, a solution can be found[12]

$$\begin{aligned} y(x) &= \left(\frac{1}{a\mathcal{D}^2 + b\mathcal{D} + c}\right)[x^3] \\ &= \left(\frac{1}{c} - \frac{b}{c^2}\mathcal{D} + \frac{b^2 - ac}{c^3}\mathcal{D}^2 - \frac{b(b^2 - 2ac)}{c^3}\mathcal{D}^3 + \mathcal{O}(\mathcal{D}^4)\right) x^3 \\ &= \frac{x^3}{c} - \frac{3bx^2}{c^2} + \frac{6(b^2 - ac)x}{c^3} - \frac{6b(b^2 - 2ac)}{c^3} \end{aligned} \tag{22-7}$$

which solves Eq. 22-6.

The Fourier transform is also a linear operator:

$$\begin{aligned} \mathcal{F}[f(x)] =& g(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{\imath kx} dx \\ \mathcal{F}^{-1}[g(k)] =& f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(k) e^{-\imath kx} dk \end{aligned} \tag{22-8}$$

Combining operators is another useful way to solve differential equations. Consider the Fourier transform, $\mathcal{F}$, operating on the differential operator, $\mathcal{D}$:

$$\mathcal{F}[\mathcal{D}[f]] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{df(x)}{dx} e^{\imath kx} dx \tag{22-9}$$

Integrating by parts,

$$= \frac{1}{\sqrt{2\pi}} f(x) \mid_{x=-\infty}^{x=\infty} - \frac{\imath k}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{\imath kx} dx \tag{22-10}$$

If the Fourier transform of $f(x)$ exists, then *typically*[13] $\lim_{x \to \pm\infty} f(x) = 0$. In this case,

$$\mathcal{F}[\mathcal{D}[f]] = -\imath k \mathcal{F}[f(x)] \tag{22-11}$$

and by extrapolation:

$$\begin{aligned} \mathcal{F}[\mathcal{D}^2[f]] &= -k^2 \mathcal{F}[f(x)] \\ \mathcal{F}[\mathcal{D}^n[f]] &= (-1)^n \imath^n k^n \mathcal{F}[f(x)] \end{aligned} \tag{22-12}$$

Operational Solutions to ODEs

Consider the heterogeneous second-order linear ODE which represent a forced, damped, harmonic oscillator that will be discussed later in this lecture.

$$M \frac{d^2 y(t)}{dt^2} + V \frac{dy(t)}{dt} + K_s y(t) = \cos(\omega_o t) \tag{22-13}$$

Apply a Fourier transform (mapping from the time (t) domain to a frequency (ω) domain) to both sides of 22-13:

$$\begin{aligned} \mathcal{F}[M \frac{d^2 y(t)}{dt^2} + V \frac{dy(t)}{dt} + K_s y(t)] &= \mathcal{F}[\cos(\omega_o t)] \\ -M\omega^2 \mathcal{F}[y] - \imath\omega V \mathcal{F}[y] + K_s \mathcal{F}[y] &= \sqrt{\frac{\pi}{2}} [\delta(\omega - \omega_o) + \delta(\omega + \omega_o)] \end{aligned} \tag{22-14}$$

[12] This method can be justified by plugging back into the original equation and verifying that the result is a solution.

[13] It is not necessary that $\lim_{x \to \pm\infty} f(x) = 0$ for the Fourier transform to exist but it is satisfied in most every case. The condition that the Fourier transform exists is that

$$\int_{-\infty}^{\infty} |f(x)| dx$$

exists and is bounded.

because the Dirac Delta functions result from taking the Fourier transform of $\cos(\omega_o t)$.

Equation 22-14 can be solved for the Fourier transform:

$$\mathcal{F}[y] = \sqrt{\frac{-\pi}{2}} \frac{[\delta(\omega - \omega_o) + \delta(\omega + \omega_o)]}{M\omega^2 + \imath\omega V - K_s} \tag{22-15}$$

In other words, the particular solution Eq. 22-13 can be obtained by finding the function $y(t)$ that has a Fourier transform equal the the right-hand-side of Eq. 22-15–or, equivalently, operating with the inverse Fourier transform on the right-hand-side of Eq. 22-15.

MATHEMATICA® does have built-in functions to take Fourier (and other kinds of) integral transforms. However, using operational calculus to solve ODEs is a bit clumsy in MATHEMATICA® . Nevertheless, it may be instructive to force it—if only as an an example of using a good tool for the wrong purpose.

Lecture 22 MATHEMATICA® Example 1

Use of Fourier Transform for Solution to the Damped-Forced Harmonic Oscillator

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A check is made to see if `FourierTransform` obeys the rules of a linear operator (Eq. 22-1) and define rule-patterns for those cases where it doesn't. Subsequently, an example the damped-forced linear harmonic oscillator is Fourier transformed, solved algebraically, and then inverse-transformed for a solution.

```
1  Table[FourierTransform[D[f[x], {x, i}], x, k], {i, 24}] //
     MatrixForm

2  FourierTransform[a f[x] + b g[x], x, k]

3  ConstantRule =
     FourierTransform[(NoX_. ) *( fun_), x_ , k_] :>
       NoX FourierTransform[fun, x, k] /;
         (FreeQ[NoX, x] && MemberQ[fun, x, Infinity])
   DistributeRule =
     FourierTransform[Plus[expr_], x_, k_] :>
       Distribute[FourierTransform[expr, x, k], Plus]

4  FourierTransform[a x f[x] + b v[x] g[x] + d p[x], x, k] //.
       DistributeRule //. ConstantRule

5  ODE2nd =
     Mass D[y[t], {t, 2}] + Viscosity D[y[t], t] + SpringK y [t]

6  FrrODE2nd =
     Factor[FourierTransform[ODE2nd, t, ω] //. DistributeRule //.
         ConstantRule]

7  rhs = FourierTransform[Cos[ ω0 t] , t, ω]

8  ftsol = Solve[FrrODE2nd == rhs, FourierTransform[y[t], t, ω]]

9  InverseFourierTransform[
     FourierTransform[y[t], t, ω] /. Flatten[ftsol],
     ω, t, Assumptions → ω0 > 0]

10 GenSol = DSolve[
       {Mass D[y[t], {t, 2}] + Damper D[y[t], t] + SpringK y[t] ==
           Cos[ωo t], y[0] == 1, y'[0] == 0}, y[t], t]

11 FullSimplify[y[t] /. Flatten[GenSol],
     Assumptions -> ω0 > 0 &&
         Mass > 0 && Damper > 0 && SpringK > 0]
```

1: As of MATHEMATICA® 5.0, `FourierTransform` automatically implements Eqs. 22-12. Here, `Table` is used to demonstrate this up to 24 derivatives.

2: However, this will demonstrate that the "sum-rule" isn't implemented automatically (n.b., although `Distribute` would implement this rule).

3: Define rules so that the FourierTransform acts as a linear functional operator. *ConstantRule* is an example of a `RuleDelayed` (`:>`) that will allow replacement with patterns that will be evaluated when the rule is applied with `ReplaceAll` (`/.`); in this case, a `Condition` (`/;`) is appended to the rule so that those cofactors which don't depend on the transformation variable, x, can be identified with `FreeQ` and those that depend on x can be identified with `MemberQ`. *DistributeRule* uses `Distribute` to replace the Fourier transform of a sum with a sum of Fourier transforms.

4: The linear rules are dispatched by a `ReplaceRepeated` (`//.`) that will continue to use the replacement until the result stops changing.

6: Apply the Fourier transform to the the left-hand-side damped-second-order ODE 22-13. . .

8: And, set the transform of the left-hand-side equal to the Fourier transform of a forcing function $\cos(\omega_o t)$. Solve for the Fourier Transform. . .

9: Back-transform the solution to find the particular solution to the damped forced second-order ODE.

11: This is the general solution obtained directly with `DSolve`; it is the solution to the homogeneous equation plus the particular solution that was obtained by the Fourier transform method.

Operators to Functionals

Equally powerful is the concept of a *functional* which takes a function as an argument and returns a value. For example $\mathcal{S}[y(x)]$, defined below, operates on a function $y(x)$ and returns its surface of revolution's area for $0 < x < L$:

$$\mathcal{S}[y(x)] = 2\pi \int_0^L y\sqrt{1+\left(\frac{dy}{dx}\right)^2}\,dx \tag{22-16}$$

This is the functional to be minimized for the question, "Of all surfaces of revolution that span from $y(x=0)$ to $y(x=L)$, which is the $y(x)$ that has the smallest surface area?"

This idea of finding "which function maximizes or minimizes something" can be very powerful and practical.

Suppose you are asked to run an "up-hill" race from some starting point $(x=0, y=0)$ to some ending point $(x=1, y=1)$ and there is a ridge $h(x,y) = x^2$. What is the most efficient running route $y(x)$?[14]

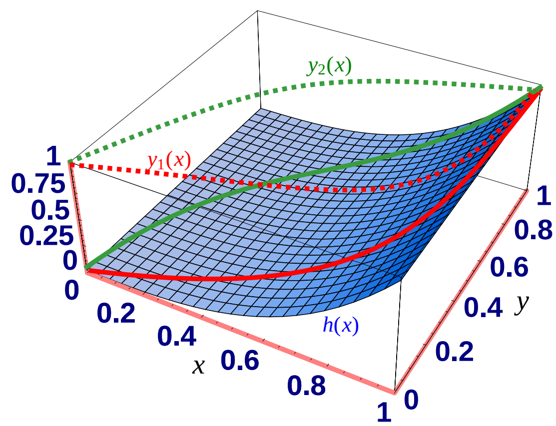

Figure 22-23: The terrain separating the starting point $(x=0, y=0)$ and ending point $(x=1, y=1)$. Assuming a model for how much running speed slows with the steepness of the path—which route would be quicker, one $(y_1(x))$ that starts going up-hill at first or another $(y_2(x))$ that initially traverses a lot of ground quickly?

A reasonable model for running speed as a function of climbing-angle α is

$$v(s) = \cos(\alpha(s)) \tag{22-17}$$

where s is the arclength along the path. The maximum speed occurs on flat ground $\alpha = 0$ and running speed monotonically falls to zero as $\alpha \rightarrow \pi/2$. To calculate the time required to traverse *any* path $y(x)$ with endpoints $y(0) = 0$ and $y(1) = 1$,

$$\begin{aligned} \frac{ds}{dt} &= v(s) = \cos(\alpha(s)) = \frac{ds}{\sqrt{ds^2+dh^2}} = \frac{1}{\sqrt{1+\frac{dh}{ds}^2}} = \frac{1}{\sqrt{1+\frac{dh^2}{dx^2+dy^2}}} \\ dt &= \frac{ds}{v(s)} = \frac{\sqrt{dx^2+dy^2}}{\cos(\alpha(s))} = \sqrt{dx^2+dy^2+dh^2} = \sqrt{1+\frac{dy}{dx}^2+\frac{dh}{dx}^2}\,dx \end{aligned} \tag{22-18}$$

[14] An amusing variation on this problem would be to find the path that the path that a winning downhill skier should traverse.

So, with the hill $h(x) = x^2$, the time as a functional of the path is:

$$\mathcal{T}[y(x)] = \int_0^1 \sqrt{1 + \frac{dy}{dx}^2 + 4x^2}\, dx \qquad (22\text{-}19)$$

There is a powerful and beautiful mathematical method for finding the extremal functions of functionals which is called *Calculus of Variations*.

By using the calculus of variations, the optimal path $y(x)$ for Eq. 22-19 can be determined:

$$y(x) = \frac{2x\sqrt{1+4x^2} + \sinh^{-1}(2x)}{2\sqrt{5} + \sinh^{-1}(2)} \qquad (22\text{-}20)$$

The approximation determined in the MATHEMATICA® example above is pretty good.

Lecture 22 MATHEMATICA® Example 2

Functionals: Introduction to Variational Calculus by Variation of Parameters

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An example of *minimizing an integral of a particular form* produced where the *variational calculus* method of minimizing over all possible functions $y(x)$ is replaced by a three-parameter family of functions $y(x; a, b, c)$.

1: Here, the "hill-function" in Eq. 22-18 specified as $h(x) = x^2$ and a three-parameter family of possible trajectories $y(x; a, b, c)$ is specified: the parameters a, b, and c, that minimize the functional subject to boundary condtiions will be determined.

2: The condition cubic equation satisfies the boundary conditions is determined using `Solve` which generates a rule that fixes two of the three free parameters.

3: By integrating $y(x)$ in Eq. 22-19, the functional equation is transformed to a function of the remaining free variable. (It is faster to do the indefinite integral evaluate the limits for the definite integral in a separate step.)

5: Plotting the time to trajectory traversal time as a function of the remaining parameter, shows there is a minimum.

6: The minimizing condition can be determined with `FindMinimum`.

7: The approximation (i.e., cubic polynomial) is fully determined by back-substitution of the mininimality condition.

9: The exact solution can be determined by a method called the *calculus of variations* and is given here.

12: The cubic polynomial is a very good approximation to the exact solution.

The problem of finding the minimizing function for the time

$$T[y(x)] = \int_{x=0}^{x=1} \sqrt{1 + \left(\frac{dy}{dx}\right)^2 + \left(\frac{dh}{dx}\right)^2}\, dx$$

for all y(x) that satisify the specified boundary condtions can be solved by the calculus of variations.
An approximation to the optimal path from the infinite set of all paths connecting $y(x=0) = 0$ to $y(x=1) = 1$ will be replaced by looking at all second-order polynomials: $y(x) = a + bx + cx^2$

```
1  h = x^2;
   YGeneral = a + b x + c x^2;
```

The general path must satisfy the boundary conditions:

```
2  YSatisifyingBCs = YGeneral /.
      (Solve[{(YGeneral /. x → 0) == 0, (YGeneral /. x → 1) == 1},
         {a, c}] // Flatten)
```

There is one remaining free variable, it can be determined by minimizing the integral

```
3  TimeInt = Integrate[
      Sqrt[1 + (D[YSatisifyingBCs, x])^2 + (D[h, x])^2], x]
4  Time = Simplify[(TimeInt /. x → 1) − (TimeInt /. x → 0)]
5  Plot[Time, {b, −2, 2}]
6  Bminsol = FindMinimum[Time, {b, 0, 1}]
7  YCubicSolution = YSatisifyingBCs /. Bminsol[[2]]
8  ApproxSolution = Plot[YCubicSolution, {x, 0, 1}]
9  YExactSolution =
      (2 x Sqrt[1 + 4 x^2] + ArcSinh[2 x]) / (2 Sqrt[5] + ArcSinh[2]);
10 Series[YExactSolution, {x, 0, 6}] // Normal // N
11 ExactSolution = Plot[YExactSolution,
      {x, 0, 1}, PlotStyle → {Thickness[0.005], Hue[1]}]
12 Show[ApproxSolution, ExactSolution]
```

Harmonic Oscillators

Methods for finding general solution to the linear inhomogeneous second-order ODE

$$a\frac{d^2y(t)}{dt^2} + b\frac{dy(t)}{dt} + cy(t) = F(t) \tag{22-21}$$

have been developed and worked out in MATHEMATICA® examples.

Eq. 22-21 arises frequently in physical models, among the most common are:

$$\begin{aligned} &\text{Electrical circuits:} && L\frac{d^2I(t)}{dt^2} + \rho l_o\frac{dI(t)}{dt} + \frac{1}{C}I(t) = V(t) \\ &\text{Mechanical oscillators:} && M\frac{d^2y(t)}{dt^2} + \eta l_o\frac{dy(t)}{dt} + K_s y(t) = F_{app}(t) \end{aligned} \tag{22-22}$$

where:

	Mechanical	Electrical
Second Order	**Mass** M: Physical measure of the ratio of momentum field to velocity	**Inductance** L: Physical measure of the ratio of stored magnetic field to current
First Order	**Drag Coefficient** $c = \eta l_o$ (η is viscosity l_o is a unit displacement): Physical measure of the ratio environmental resisting forces to velocity—or proportionality constant for energy dissipation with square of velocity	**Resistance** $R = \rho l_o$ (ρ is resistance per unit material length l_o is a unit length): Physical measure of the ratio of voltage drop to current—or proportionality constant for power dissipated with square of the current.
Zeroth Order	**Spring Constant** K_s: Physical measure of the ratio environmental force developed to displacement—or proportionality constant for energy stored with square of displacement	**Inverse Capacitance** $1/C$: Physical measure of the ratio of voltage storage rate to current—or proportionality constant for energy storage rate dissipated with square of the current.
Forcing Term	**Applied Voltage** $V(t)$: Voltage applied to circuit as a function of time.	**Applied Force** $F(t)$: Force applied to oscillator as a function of time.

For the homogeneous equations (i.e. no applied forces or voltages) the solutions for physically allowable values of the coefficients can either be oscillatory, oscillatory with damped amplitudes, or, completely damped with no oscillations. (See Figure 21-21). The homogeneous equations are sometimes called *autonomous* equations—or *autonomous systems*.

Simple Undamped Harmonic Oscillator

The simplest version of a homogeneous Eq. 22-21 with no damping coefficient ($b = 0$, $R = 0$, or $\eta = 0$) appears in a remarkably wide variety of physical models. This simplest physical model is a simple harmonic oscillator—composed of a mass accelerating with a linear spring restoring force:

$$\begin{aligned} \text{Inertial Force} &= \text{Restoring Force} \\ M\text{Acceleration} &= \text{Spring Force} \\ M\frac{d^2y(t)}{dt^2} &= -K_s y(t) \\ M\frac{d^2y(t)}{dt^2} + K_s y(t) &= 0 \end{aligned} \tag{22-23}$$

Here y is the displacement from the equilibrium position–i.e., the position where the force, $F = -dU/dx = 0$. Eq. 22-23 has solutions that oscillate in time with frequency ω:

$$\begin{aligned} y(t) &= A\cos\omega t + B\sin\omega t \\ y(t) &= C\sin(\omega t + \phi) \end{aligned} \tag{22-24}$$

where $\omega = \sqrt{K_s/M}$ is the natural frequency of oscillation, A and B are integration constants written as amplitudes; or, C and ϕ are integration constants written as an amplitude and a phase shift.

The simple harmonic oscillator has an *invariant*, for the case of mass-spring system the invariant is the total energy:

$$
\begin{aligned}
\text{Kinetic Energy} + \text{Potential Energy} &= \\
\frac{M}{2}v^2 + \frac{K_s}{2}y^2 &= \\
\frac{M}{2}\frac{dy}{dt}^2 + \frac{K_s}{2}y^2 &= \\
A^2\omega^2\frac{M}{2}\cos^2(\omega t + \phi) + A^2\frac{K_s}{2}\sin^2(\omega t + \phi) &= \\
A^2(\omega^2\frac{M}{2}\cos^2(\omega t + \phi) + \frac{M\omega^2}{2}\sin^2(\omega t + \phi) &= \\
A^2 M\omega^2 &= \text{constant}
\end{aligned}
\qquad (22\text{-}25)
$$

There are a remarkable number of physical systems that can be reduced to a simple harmonic oscillator (i.e., the model can be reduced to Eq. 22-23). Each such system has an analog to a mass, to a spring constant, and thus to a natural frequency. Furthermore, every such system will have an invariant that is an analog to the total energy—an in many cases the invariant will, in fact, be the total energy.

The advantage of reducing a physical model to a harmonic oscillator is that *all of the physics follows from the simple harmonic oscillator.*

Here are a few examples of systems that can be reduced to simple harmonic oscillators:

Pendulum By equating the rate of change of angular momentum equal to the torque, the equation for pendulum motion can be derived:

$$MR^2\frac{d^2\theta}{dt^2} + MgR\sin\theta = 0 \qquad (22\text{-}26)$$

for small-amplitude pendulum oscillations, $\sin(\theta) \approx \theta$, the equation is the same as a simple harmonic oscillator.

It is instructive to consider the invariant for the non-linear equation. Because

$$\frac{d^2\theta}{dt^2} = \frac{d\theta}{dt}\left(\frac{d\frac{d\theta}{dt}}{d\theta}\right) \qquad (22\text{-}27)$$

Eq. 22-26 can be written as:

$$MR^2\frac{d\theta}{dt}\left(\frac{d\frac{d\theta}{dt}}{d\theta}\right) + MgR\sin(\theta) = 0 \qquad (22\text{-}28)$$

$$\frac{d}{d\theta}\left[\frac{MR^2}{2}\left(\frac{d\theta}{dt}\right)^2 - MgR\cos(\theta)\right] = 0 \tag{22-29}$$

which can be integrated with respect to θ:

$$\frac{MR^2}{2}\left(\frac{d\theta}{dt}\right)^2 - MgR\cos(\theta) = \text{constant} \tag{22-30}$$

This equation will be used as a level-set equation to visualize pendulum motion.

Buoyant Object Consider a buoyant object that is slightly displaced from its equilibrium floating position. The force (downwards) due to gravity of the buoy is $\rho_{bouy} g V_{bouy}$ The force (upwards) according to Archimedes is $\rho_{water} g V_{sub}$ where V_{sub} is the volume of the buoy that is submerged. The equilibrium position must satisfy $V_{sub-eq}/V_{bouy} = \rho_{bouy}/\rho_{water}$.

If the buoy is slightly perturbed at equilibrium by an amount δx the force is:

$$\begin{aligned} F =& \rho_{water} g (V_{sub-eq} + \delta x A_o) - \rho_{buoy} g V_{buoy} \\ F =& \rho_{water} g \delta x A_o \end{aligned} \tag{22-31}$$

where A_o is the cross-sectional area at the equilibrium position. Newton's equation of motion for the buoy is:

$$M_{buoy}\frac{d^2y}{dt^2} - \rho_{water} g A_o y = 0 \tag{22-32}$$

so the characteristic frequency of the buoy is $\omega = \sqrt{\rho_{water} g A_o / M_{bouy}}$.

Single Electron Wave-function The one-dimensional Schrödinger equation is:

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left(E - U(x)\right)\psi = 0 \tag{22-33}$$

where $U(x)$ is the potential energy at a position x. If $U(x)$ is constant as in a free electron in a box, then the one-dimensional wave equation reduces to a simple harmonic oscillator.

In summation, just about any system that oscillates about an equilibrium state can be reduced to a harmonic oscillator.