Separation of Variables in Linear PDE

Now we apply the theory of Hilbert spaces to linear differential equations with partial derivatives (PDE). We start with a particular example, the one-dimensional (1D) wave equation

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} \ , \tag{1}$$

where physical interpretations of the function $u \equiv u(x,t)$ (of coordinate x and time t), and the velocity, c, depend on a particular problem. To be specific, we can think of u as a perpendicular displacement of a string in xy plane, attached by two ends; the x axis is along the string. Without loss of generality, we set $c = 1$, since this just corresponds to properly re-scaling t. The fact that the two ends, $x = a$ and $x = b$, of the string are fixed is expressed by the boundary conditions:

$$u(a,t) = u(b,t) = 0 \ . \tag{2}$$

We also need to specify particular initial conditions for the function and its time derivative:

$$u(x,0) = g_1(x) \ , \qquad \dot{u}(x,0) = g_2(x) \ . \tag{3}$$

Note an asymmetry between the variables x and t. With respect to t we have a Cauchy-type problem with initial conditions, while with respect to x we are dealing with a boundary value problem. That is why we will treat x and t differently. With respect to the variable x, we will look at $u(x,t)$ as if it is a vector of the space $\mathcal{L}_2[a,b]$ (that depends on t as a parameter):

$$u(x,t) \equiv |u(t)\rangle \ . \tag{4}$$

In the vector notation, Eq. (74) has the form

$$\frac{d^2}{dt^2}|u(t)\rangle = L|u(t)\rangle \ , \tag{5}$$

where L is a linear operator—in our case $L = \Delta \equiv \partial^2/\partial x^2$ is the Laplace operator.

The following circumstances are crucial:

(i) Within the space $\mathcal{L}_2[a,b]$ we can introduce a *subspace* $\tilde{\nu}$ of functions that have second derivatives and satisfy the conditions (2).

(ii) The subspace $\tilde{\nu}$ is dense in $\mathcal{L}_2[a,b]$, which means that any vector in $\mathcal{L}_2[a,b]$ can be approximated with any given accuracy by a vector from $\tilde{\nu}$, and, correspondingly, any orthonormal basis (ONB) in $\tilde{\nu}$ is automatically an ONB for the whole Hilbert space $\mathcal{L}_2[a,b]$.

(iii) Operator L is well-defined and self-adjoint in $\tilde{\nu}$, and thus there exists an ONB consisting of the eigenvectors of L.

Comments. The fact that $\tilde{\nu}$ is a vector space is easily seen. The statement that Laplace operator $\Delta = \partial^2/\partial x^2$ is self-adjoint in $\tilde{\nu}$ is checked by doing integrals by parts with (2) taken into account (we use sub-script notation for partial derivatives):

$$\langle f|\Delta|g\rangle = \int_a^b f^* g_{xx}\, dx = f^* g_x\,|_a^b - \int_a^b f_x^* g_x\, dx =$$

$$= f^* g_x\,|_a^b - f_x^* g\,|_a^b + \int_a^b f_{xx}^* g\, dx = \int_a^b f_{xx}^* g\, dx = \langle \Delta f|g\rangle \,. \tag{6}$$

Here f and g are two functions belonging to $\tilde{\nu}$, which by definition means that they obey the boundary conditions (2), and thus the boundary terms in (6) are equal to zero.

We have already discussed that two eigenvectors of a self-adjoint linear operator are automatically orthogonal if they correspond to different eigenvalues. The eigenvectors of one and the same eigenvalue are not necessarily orthogonal, but they form a vector subspace and thus can be orthonormalized by Gram-Schmidt procedure.

It is a serious problem, however, to prove the completeness of the system of eigenvectors of a Hermitian operator in an infinite-dimensional space. The proof goes beyond the present course, and below we will be taking for granted—trusting our mathematician colleagues—that for any self-adjoint differential operator there exists an orthonormalized eigenvector set that forms an ONB in $\mathcal{L}_2[a,b]$.

Once we know that there exists an ONB of eigenvectors of Δ, we can find these vectors explicitly by just solving the second-order ordinary differential equation

$$e''(x) = \lambda\, e(x) \,, \tag{7}$$

with proper boundary conditions, which in our case are

$$e(a) = e(b) = 0 \,. \tag{8}$$

The general solution of (7) is a sine/cosine function for a negative λ,

$$e(x) = A \sin(x\sqrt{-\lambda} + \theta_0) \qquad (\lambda < 0) , \qquad (9)$$

an exponential function for a positive λ,

$$e(x) = B\mathrm{e}^{x\sqrt{\lambda}} + C\mathrm{e}^{-x\sqrt{\lambda}} \qquad (\lambda > 0) \qquad (10)$$

and a linear function for $\lambda = 0$,

$$e(x) = D + Ex \qquad (\lambda = 0) . \qquad (11)$$

With an exponential function, however, the only way to satisfy the boundary conditions is to have $B = C = 0$, which is a trivial solution (zero vector). In the case of $\lambda = 0$ the solution is also trivial: $D = E = 0$.

Hence, all the eigenvalues are negative, and we need to examine the solution (9). Without loss of generality, set $a = 0$ and $b = 1$.—This can be always achieved by shifting and re-scaling x. Then

$$e(0) = 0 \qquad \Rightarrow \qquad \sin \theta_0 = 0 \qquad \Rightarrow \qquad \theta_0 = 0 . \qquad (12)$$

(The solution $\theta_0 = \pi$ corresponds to just changing the sign of A.) Now we need to satisfy the second boundary condition:

$$e(1) = 0 \qquad \Rightarrow \qquad \sin(\sqrt{-\lambda}) = 0 \qquad \Rightarrow \qquad \sqrt{-\lambda} = \pi m , \qquad (13)$$

where m is an integer. Noting that $m \to -m$ does not produce a new linear independent vector, we have to confine ourselves to $m > 0$. Hence,

$$\lambda_m = -\pi^2 m^2 , \qquad m = 1, 2, 3, \ldots . \qquad (14)$$

The eigenfunctions are

$$e_m(x) \propto \sin(\pi m x) , \qquad m = 1, 2, 3, \ldots . \qquad (15)$$

They are automatically orthogonal, since there is only one function for any eigenvalue. The normalization condition is

$$\int_0^1 e_m^2(x) \, dx = 1 , \qquad (16)$$

and we finally get

$$e_m(x) = \sqrt{2} \sin(\pi m x) , \qquad m = 1, 2, 3 \ldots . \qquad (17)$$

Now we have an ONB and can look for a solution of the vector equation (5) in the form of the expansion

$$|u(t)\rangle \;=\; \sum_{m=1}^{\infty} u_m(t) \,|e_m\rangle \;, \tag{18}$$

where $u_m(t)$ are time-dependent Fourier coefficients. We plug this into (5) and (3) and form an inner product with an eigenvector $|e_m\rangle$. Taking advantage of the fact that we are dealing with the eigenvectors of the operator L, we get

$$\ddot{u}_m(t) = \lambda_m u_m(t) \;, \tag{19}$$

with

$$u_m(0) = \langle e_m|g_1\rangle = \int_0^1 e_m(x)\, g_1(x)\, dx \;, \tag{20}$$

$$\dot{u}_m(0) = \langle e_m|g_2\rangle = \int_0^1 e_m(x)\, g_2(x)\, dx \;. \tag{21}$$

For each $u_m(t)$ we have an *independent* equation (19)—an ordinary second-order differential equation—with the initial conditions given by (20) and (48).

Since all λ's are negative, each of Eqs. (19) is just a harmonic oscillator with the frequency

$$\omega_m \;=\; \sqrt{-\lambda_m} \;=\; \pi m \;. \tag{22}$$

We have already considered this problem in our course, and thus just write down the answer satisfying given initial conditions:

$$u_m(t) = u_m(0)\cos(\omega_m t) \;+\; (\dot{u}_m(0)/\omega_m)\sin(\omega_m t) \;, \tag{23}$$

where for each m the values of $u_m(0)$ and $\dot{u}_m(0)$ are obtained by doing integrals (20) and (48), respectively. The solution to the whole problem thus reads:

$$u(x,t) \;=\; \sum_{m=1}^{\infty} \left[A_m \cos(\pi m t) \;+\; B_m \sin(\pi m t)\right] \sin(\pi m x) \;, \tag{24}$$

$$A_m \;=\; 2\int_0^1 g_1(x)\sin(\pi m x)dx \;, \tag{25}$$

$$B_m \;=\; (2/\pi m)\int_0^1 g_2(x)\sin(\pi m x)dx \;. \tag{26}$$

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The solution (24) has the form of a sum of products of functions of t and x. In this connection, the method is often referred to as the method of separation of variables—x and t in our case. Note, however, that x and t were treated absolutely differently.

Heat equation. Now consider the heat equation

$$\frac{\partial u}{\partial t} = \kappa \frac{\partial^2 u}{\partial x^2} + f , \tag{27}$$

where $u \equiv u(x,t)$ is the temperature as a function of coordinate x and time t; the parameter $\kappa > 0$ is the thermal diffusivity; $f \equiv f(x,t)$ is the heat transferred to (if $f > 0$)/removed from (if $f < 0$) the system per unit time and per unit length. [Below we set $\kappa = 1$, which can always be done by rescaling t and f.] We assume that our system is finite: $x \in [a,b]$. To complete the statement of the problem, we need the initial condition

$$u(x,0) = g(x) , \tag{28}$$

and the boundary conditions at $x = a$ and $x = b$. To be specific, we assume that our system is thermally isolated at both ends. This means that there is no heat flow at $x = a$ and $x = b$, and—since the heat flow is proportional to the temperature gradient—we have

$$u_x(a,t) = u_x(b,t) = 0 . \tag{29}$$

Here we use a convenient notation $u_x \equiv \partial u/\partial x$.

   Mathematically, the procedure is quite similar to what we did with the wave equation. We identify the function $u(x,t)$ and $f(x,t)$ with (time-dependent) vectors:

$$u(x,t) \equiv |u(t)\rangle , \qquad f(x,t) \equiv |f(t)\rangle . \tag{30}$$

In the vector notation, Eq. (27) has the form

$$\frac{d}{dt} |u(t)\rangle = L |u(t)\rangle + |f(t)\rangle , \tag{31}$$

where $L = \Delta \equiv \partial^2/\partial x^2$ is the Laplace operator.

Once again we identify the crucial circumstances:
(i) Within the space $\mathcal{L}_2[a,b]$ one can introduce a *subspace* $\tilde{\nu}$ of functions that

have second derivatives and satisfy the conditions (29).

(ii) The subspace $\tilde{\nu}$ is dense in $\mathcal{L}_2[a, b]$, which means that any vector in $\mathcal{L}_2[a, b]$ can be approximated with any given accuracy by a vector from $\tilde{\nu}$, and, correspondingly, any orthonormal basis (ONB) in $\tilde{\nu}$ is automatically an ONB for the whole Hilbert space $\mathcal{L}_2[a, b]$.

(iii) Operator L is well-defined and self-adjoint in $\tilde{\nu}$, and thus there exists an ONB consisting of the eigenvectors of L.

The fact that $\tilde{\nu}$ is a vector space is readily seen. The statement that Laplace operator $\Delta = \partial^2/\partial x^2$ is self-adjoint in $\tilde{\nu}$ is checked by doing integrals by parts with (29) taken into account (we use shorthand notation for partial derivatives):

$$\langle f | \Delta | g \rangle = \int_a^b f^* g_{xx} \, dx = f^* g_x \big|_a^b - \int_a^b f_x^* g_x \, dx =$$

$$= f^* g_x \big|_a^b - f_x^* g \big|_a^b + \int_a^b f_{xx}^* g \, dx = \int_a^b f_{xx}^* g \, dx = \langle \Delta f | g \rangle \,. \qquad (32)$$

Here f and g are two functions from $\tilde{\nu}$. They obey the boundary conditions (29), and thus the boundary terms in (32) are equal to zero.

Now we construct an ONB of eigenvectors of Δ by solving the second-order ordinary differential equation

$$e''(x) = \lambda \, e(x) \,, \qquad (33)$$

with proper boundary conditions, which in our case are

$$e'(a) = e'(b) = 0 \,. \qquad (34)$$

The general solution of (33) is a sine/cosine function for a negative λ,

$$e(x) = A \cos(x\sqrt{-\lambda} + \theta_0) \qquad (\lambda < 0) \,, \qquad (35)$$

an exponential function for a positive λ,

$$e(x) = B \mathrm{e}^{x\sqrt{\lambda}} + C \mathrm{e}^{-x\sqrt{\lambda}} \qquad (\lambda > 0) \qquad (36)$$

and a linear function for $\lambda = 0$,

$$e(x) = D + Ex \qquad (\lambda = 0) \,. \qquad (37)$$

With an exponential function, however, the only way to satisfy the boundary conditions is to have $B = C = 0$, which is a trivial solution (zero vector).

In the case of $\lambda = 0$ we do have a non-trivial eigenvector: $E = 0$, $D \neq 0$. Hence, all the eigenvalues except for $\lambda_0 = 0$ are negative, and we need to examine the solution (35) to find them with corresponding eigenvectors. For definiteness, set $a = 0$ and $b = 1$. Then

$$e'(0) = 0 \qquad \Rightarrow \qquad \sin\theta_0 = 0 \qquad \Rightarrow \qquad \theta_0 = 0 \ . \qquad (38)$$

(The solution $\theta_0 = \pi$ corresponds to just changing the sign of A.) Now we need to satisfy the second boundary condition:

$$e'(1) = 0 \qquad \Rightarrow \qquad \sin(\sqrt{-\lambda}) = 0 \qquad \Rightarrow \qquad \sqrt{-\lambda} = \pi m \ , \qquad (39)$$

where m is an integer. Noting that $m \to -m$ does not produce a new linear independent vector, we have to confine ourselves to $m \geq 0$. Hence,

$$\lambda_m = -\pi^2 m^2 \ , \qquad m = 0, 1, 2, \dots \ . \qquad (40)$$

The eigenfunctions are

$$e_m(x) \propto \cos(\pi m x) \ , \qquad m = 0, 1, 2, \dots \ . \qquad (41)$$

They are automatically orthogonal, since there is only one function for any eigenvalue. The normalization condition is

$$\int_0^1 e_m^2(x) \, dx = 1 \ , \qquad (42)$$

and we finally get

$$e_0(x) = 1 \ , \qquad (43)$$

$$e_m(x) = \sqrt{2}\cos(\pi m x) \ , \qquad m = 1, 2, 3 \dots \ . \qquad (44)$$

Now we have an ONB and can look for a solution of the vector equation (31) in the form of the expansion

$$|u(t)\rangle = \sum_{m=0}^{\infty} u_m(t) \, |e_m\rangle \ , \qquad (45)$$

where $u_m(t)$ are time-dependent Fourier coefficients. We plug this into (31) and (28) and form an inner product with an eigenvector $|e_m\rangle$. Taking advantage of the fact that we are dealing with the eigenvectors of the operator L, we get

$$\dot{u}_m(t) = \lambda_m u_m(t) + f_m(t) \ , \qquad (46)$$

where

$$f_m(t) = \langle e_m | f \rangle = \int_0^1 e_m(x)\, f(x,t)\, dx \,, \tag{47}$$

and

$$u_m(0) = \langle e_m | g \rangle = \int_0^1 e_m(x)\, g(x)\, dx \,. \tag{48}$$

For each $u_m(t)$ we have an *independent* equation (46)—an ordinary first-order differential equation—with the initial condition (48).

For simplicity, consider the case $f = 0$. The solution for u_m is

$$u_m(t) = u_m(0)\, e^{\lambda_m t} \,, \tag{49}$$

and we ultimately have

$$u(x,t) = g_0 + \sum_{m=1}^{\infty} g_m\, e^{-\pi^2 m^2 t}\, \cos(\pi m x) \,, \tag{50}$$

$$g_0 = \int_0^1 g(x)\, dx \,, \tag{51}$$

$$g_m = 2 \int_0^1 g(x)\, \cos(\pi m x)\, dx \,, \qquad m = 1, 2, 3, \ldots \tag{52}$$

Consider now the case of time-independent $f \equiv f(x)$, and find the asymptotic solution at $t \to \infty$. For any $m > 0$ the asymptotic solution of Eq. (46) is time-independent:

$$0 = \lambda_m u_m + f_m \qquad \Rightarrow \qquad u_m = -f_m/\lambda_m \qquad (m > 0)\,. \tag{53}$$

The case of $m = 0$ is a special one, since $\lambda_0 = 0$. Here we have

$$\dot{u}_0(t) = f_0 \qquad \Rightarrow \qquad u_0(t) = g_0 + f_0\, t \,. \tag{54}$$

If $f_0 \equiv \int_0^1 f(x) dx = 0$, then u_0 is time-independent and is equal to g_0—it just remembers its initial condition. But if $f_0 \neq 0$, then, asymptotically, there is a linear increase/decrease of u_0.

We can summarize the above-discussed treatment of linear partial differential equations with Hermitian differential operator in the following algorithm.

Step 1.—Not necessary, but strongly recommended. Shift and/or rescale the variable x in such a way that $[a, b] \to [0, 1]$, or $[a, b] \to [-1, 1]$. Rescale the variable t so that to remove (reduce the number of) dimensional constants (like κ, c^2, etc.).

Step 2. Check whether the boundary conditions are canonical or not. Canonical boundary conditions imply that (i) the set of functions obeying them is a vector space, (ii) spatial differential operator is a Hermitian operator in this vector space.

If boundary conditions are not canonical, render them canonical by substituting $u(x, t) = \tilde{u}(x, t) + u_1(x, t)$ with an appropriate $u_1(x, t)$.

Step 3. Construct eigenvector ONB and find corresponding eigenvalues of the spatial differential operator. Make sure that there is no double counting of one and the same eigenvector. If there are more than one vectors corresponding to one and the same eigenvalue, and these are not orthogonal, orthonormalize them by Gram-Schmidt procedure.

Step 4. Look for the solution of the given PDE in the form of the Fourier series with respect to obtained ONB.—Plug the expansion into PDE, take into account that the basis vectors are the eigenvectors of the spatial differential operator, and form the inner products of the l.h.s. and r.h.s. of PDE with the basis vectors. This will yield an independent ordinary differential equation for each Fourier coefficient as a function of time.

If there is no time-dependence, the equations are just algebraic ones. Solve them and go directly to the step 7.

Step 5. Obtain the initial conditions for these differential equations by forming inner products of the basis vectors with the initial condition(s).

Step 6. Solve the differential equations with the initial conditions.

Step 7. Write down the answer. Restore original units of t and x, if necessary.

Problem 19. Consider the heat equation

$$u_t = u_{xx} \, , \tag{55}$$

$u = u(x, t)$, $x \in [0, 1]$, with the boundary conditions (note the derivative in the first one)

$$u_x(0, t) = 0 \, , \qquad u(1, t) = 0 \tag{56}$$

and the initial condition

$$u(x, 0) = 1 .\tag{57}$$

(a) Make sure that the boundary conditions are canonical.
(b) Construct the orthonormal basis of the eigenfunctions of the Laplace operator in the space of functions obeying the boundary conditions (56).
(c) Find the solution $u(x, t)$ of the problem (55)-(57) in the form of the Fourier series in terms of the constructed ONB.

Problem 20. Find the solution $u(x)$, $x \in [0, 1]$—in the form of the Fourier series in terms of the eigenfunctions of the Laplace operator—of the stationary heat equation

$$u_{xx} + f(x) = 0 ,\tag{58}$$

$$f(x) = \begin{cases} 1 , & x \in [0, \ 0.5) , \\ 0 , & x \in [0.5, \ 1] , \end{cases}\tag{59}$$

$$u(0) = u(1) = 0 .\tag{60}$$

Problem 21. The wavefunction $\psi(x, t)$ of a 1D quantum particle living on a ring of circumference L obeys Schrödinger equation

$$i\hbar\psi_t = -\frac{\hbar^2 \psi_{xx}}{2m} , \qquad x \in [0, \ L] ,\tag{61}$$

with periodic boundary conditions (because of the ring topology):

$$\psi(0, t) = \psi(L, t) \qquad \psi_x(0, t) = \psi_x(L, t) .\tag{62}$$

At $t = 0$ the wavefunction is

$$\psi(x, 0) = \begin{cases} (2/L)^{1/2} , & x \in [0, \ L/2] , \\ 0 , & x \in (L/2, \ L) . \end{cases}\tag{63}$$

Solve for $\psi(x, t)$. Do not forget that in contrast to heat and wave equations, the function ψ is complex.

Now we would like to generalize the above-discussed treatment. There are three issues to be addressed: (i) the form of the time-differential term, (ii) the form of the differential operator L, and (iii) the form of the boundary conditions under which we can introduce a vector subspace $\tilde{\nu}$ for the solutions with the operator L being Hermitian for all $|u\rangle \in \tilde{\nu}$.

Form of the time-differential term. The only requirement here is that this

term is linear.—Otherwise, the series expansion makes little sense. Hence, we can work with any equation of the form

$$\mathcal{D}\,|u(t)\rangle \;=\; L\,|u(t)\rangle + |f(t)\rangle \;, \tag{64}$$

where $\mathcal{D}$ is *any* linear time-differential operator, or just zero.

Sturm-Liouville operator. The general form of a second-order real differential operator which proves Hermitian under appropriate boundary conditions is as follows.

$$L = \frac{1}{w(x)}\left[\frac{\partial}{\partial x}\,p(x)\,\frac{\partial}{\partial x} - q(x)\right] \;, \tag{65}$$

where w, p, and q are real, and also $w > 0$. It is the Sturm-Liouville operator. The inner product now is defined with the weight function $w(x)$, and that is why we need the requirement $w > 0$. Doing the integrals by parts—in complete analogy with Eq. (6)—we get

$$\langle f|L|g\rangle \;=\; pf^*g_x\big|_a^b - pf_x^*g\big|_a^b + \langle Lf|g\rangle \;. \tag{66}$$

We see that the operator L is Hermitian in the subspace $\tilde{\nu}$ if for any $|f\rangle$, $|g\rangle \in \tilde{\nu}$ the boundary terms in the r.h.s. of (66) are zero. This can be achieved if $\forall\,|f\rangle \in \tilde{\nu}$ the following condition is satisfied

$$[\,(f(a)=0)\ \textbf{ or }\ (f_x(a)=0)\ \textbf{ or }\ (f_x(a)/f(a)=\xi_a)\ \textbf{ or }\ (p(a)=0)\,]\quad \textbf{and}$$

$$[\,(f(b)=0)\ \textbf{ or }\ (f_x(b)=0)\ \textbf{ or }\ (f_x(b)/f(b)=\xi_b)\ \textbf{ or }\ (p(b)=0)\,]\;. \tag{67}$$

Here ξ_a and ξ_b are f-independent constants. In the case $p(a)=0$ $[p(b)=0]$ the boundary condition also implies that $f(a)$ $[f(b)]$ is finite at $x \to a$ $[x \to b]$, and this is indeed a *condition*, because in this case divergent solutions appear. This boundary condition excludes them.

The operator L is Hermitian also in the *periodic* case:

$$p(a)=p(b), \quad f(a)=f(b), \quad f_x(a)=f_x(b)\;. \tag{68}$$

We will refer to the boundary conditions (67) and (68) as *canonical*. If either (67) or (68) takes place, the eigenfunctions $e_j(x)$ and eigenvalues λ_j of the operator L are found by solving the Sturm-Liouville equation

$$\frac{\partial}{\partial x}\,p\,\frac{\partial u}{\partial x} - qu = \lambda w u \;. \tag{69}$$

Note (check) that *any* operator

$$L \;=\; r(x)\,\frac{\partial^2}{\partial x^2} + s(x)\,\frac{\partial}{\partial x} + z(x) \tag{70}$$

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with real r, s, z and $s, r > 0$ can be written in the form (65), with

$$p(x) = \exp\left[\int_a^x dx'\, s(x')/r(x')\right] , \qquad w = p/r , \quad q = -zw . \qquad (71)$$

Below we list some characteristic 1D equations which can be solved by the method described above under the canonical boundary conditions.

$$u_t = \kappa u_{xx} + f(x,t) \qquad \text{(Heat/diffusion equation)}, \qquad (72)$$

$$iu_t = -u_{xx} + q(x)\,u \qquad \text{(Schrödinger equation)} \qquad (73)$$

(we use the units $\hbar = 2m = 1$),

$$u_{tt} = c^2 u_{xx} + f(x,t) \qquad \text{(Wave equation)}, \qquad (74)$$

where c is the wave velocity and f is an external force, and

$$u_{xx} = f(x) \qquad \text{(Poisson equation)} . \qquad (75)$$

Non-canonical boundary conditions. If the boundary conditions are non-canonical, then a generic prescription is to subtract from the function $u(x,t)$ some particular function $u_1(x,t)$, so that the difference $\tilde{u}(x,t) = u(x,t) - u_1(x,t)$ satisfies one of the canonical boundary conditions. Clearly, this subtraction will result only in changing the form of the function $f(x,t)$. We illustrate this idea by the following example. Let

$$u(a,t) = \mu(t) , \qquad u_x(b,t) = \eta(t) . \qquad (76)$$

Now if we write

$$u(x,t) = \tilde{u}(x,t) + u_1(x,t) , \qquad (77)$$

where

$$u_1(x,t) = \mu(t) + (x-a)\,\eta(t) , \qquad (78)$$

then for the function $\tilde{u}(x,t)$ we get

$$\tilde{u}(a,t) = 0 , \qquad \tilde{u}_x(b,t) = 0 , \qquad (79)$$

which are the canonical boundary conditions. In particular, if $u(x,t)$ is supposed to satisfy the heat equation

$$u_t = u_{xx} + f , \qquad (80)$$

then for the function $\tilde{u}$ we will have

$$\tilde{u}_t = \tilde{u}_{xx} + \tilde{f} \ , \tag{81}$$

with

$$\tilde{f}(x,t) = f(x,t) + \frac{\partial^2 u_1}{\partial x^2} - \frac{\partial u_1}{\partial t} \ . \tag{82}$$

That is

$$\tilde{f}(x,t) = f(x,t) - \dot{\mu}(t) - (x - a)\,\dot{\eta}(t) \ . \tag{83}$$

Issues of Convergence. Gibbs Phenomenon

When constructing ONB of eigenfunctions of Sturm-Liouville operator, we are dealing with a vector space $\tilde{\nu}$ defined by the (canonical) boundary conditions of a given equation. Is this requirement really crucial? Indeed, *any* ONB in the Hilbert space $\mathcal{L}_2[a,b]$ can be used for expanding *any* function $\mathcal{L}_2[a,b]$. So why don't we use ONB corresponding to, say, periodic boundary conditions for expanding a function u satisfying the conditions $u(a) = 0$, $u_x(b) = 0$, or vice versa?

The point is that the convergence in this case will be, generally speaking, *almost* everywhere, rather than every where. And this is really crucial, because the central step of the algorithm of solving PDE is the interchanging the orders of summation and differentiation when acting with the Sturm-Liouville operator on the Fourier series. This is legitimate only if the series converges everywhere rather than almost everywhere.

Gibbs phenomenon. Consider the solution (50)-(52) to the problem (27)-(29) in the case when the initial condition reads

$$g(x) = \begin{cases} 1 \ , & x \in [0, \ 0.5] \ , \\ 0 \ , & x \in (0.5, \ 1] \ . \end{cases} \tag{84}$$

A comment is in order here concerning the consistency of this *discontinuous* initial condition with PDE implying existence of the derivatives. Actually, the initial condition (84) is understood as a limit of a smooth, but arbitrarily steep function. And the solution (50)-(52) is just what we need for taking this limit, since it contains only the *integrals* of the function $g(x)$, which are well defined even for a discontinuous function.

Even if the evolution of $u(x)$ starts from a stepwise initial condition (84), at any finite t the solution is smooth. However, the convergence of the series towards this smooth solution is rather peculiar. Let us explore this convergence. Explicitly doing the integrals, we get

$$g_0 = 1/2 \;, \tag{85}$$

$$g_m = \int_0^{1/2} \cos(\pi m x)\, dx \;=\; \begin{cases} (-1)^n/\pi m \;, & m = 2n + 1 \;, \\ 0 \;, & m = 2n \end{cases} \tag{86}$$

[here n is integer] and arrive at the final answer

$$u(x,t) \;=\; 1/2 + (2/\pi) \sum_{n=0}^{\infty} \frac{(-1)^n}{2n+1}\; e^{-\pi^2(2n+1)^2 t}\; \cos[(2n+1)\pi x] \;. \tag{87}$$

In Figs. 1 and 2 we plot some partial sums of the series (87), with $n_{\max}$ being the maximal n in the sum. We see that at $t = 0$ the convergence is not homogeneous: No matter how large is $n_{\max}$, there is always a *finite amplitude* overshoot in the vicinity of the point $x = 0.5$. Such an overshoot is generic for Fourier expansions of stepwise functions. It is called Gibbs phenomenon. In Fig. 2 we present truncated series at a very small, but finite t. We see a qualitative difference. While at small enough $n_{\max}$ the result is indistinguishable from that of $t = 0$, at larger $n_{\max}$ Gibbs phenomenon disappears.

A similar situation with Gibbs phenomenon arises when the initial condition does not satisfy one or both boundary conditions. See, for example, problem 20. The solution will satisfy the boundary conditions at any $t > 0$, but not at $t = 0$. Correspondingly, at the boundary at which the boundary condition is not satisfied at $t = 0$, the Gibbs phenomenon in the Fourier series (but not in real life!) will be seen in the limit of small enough times.
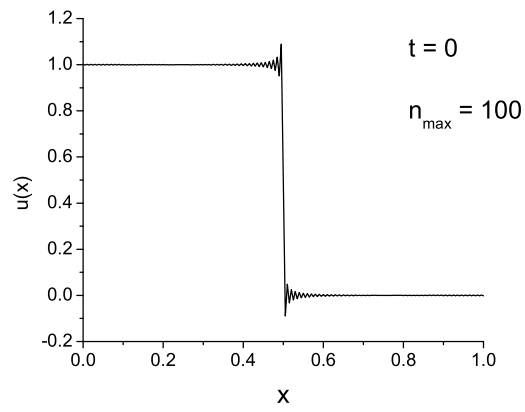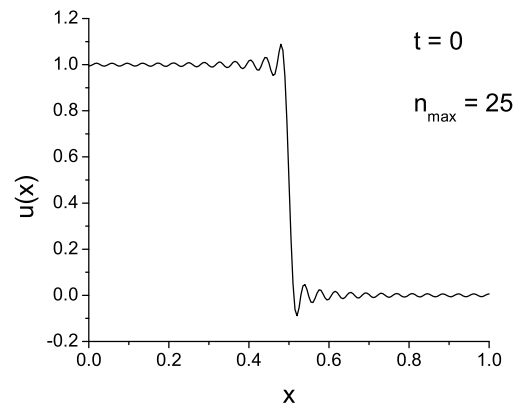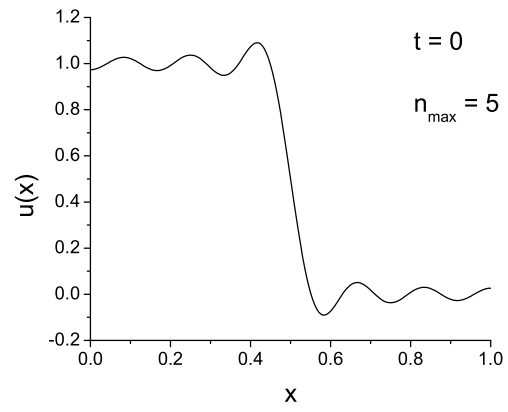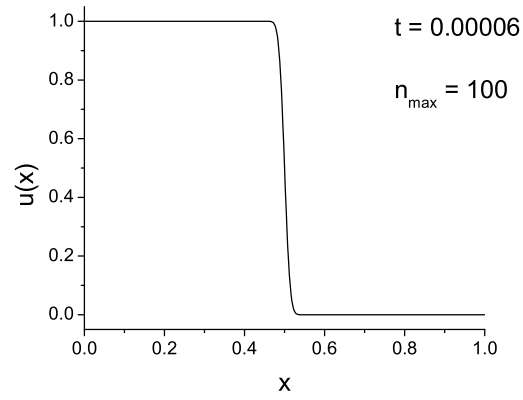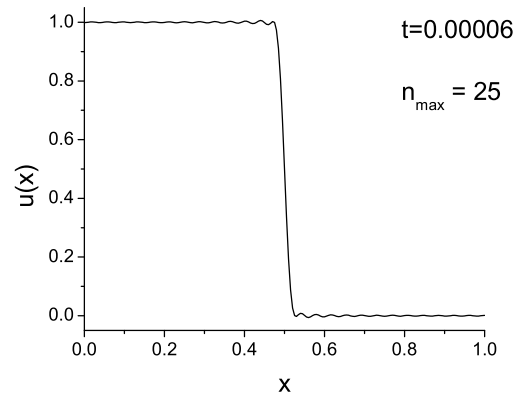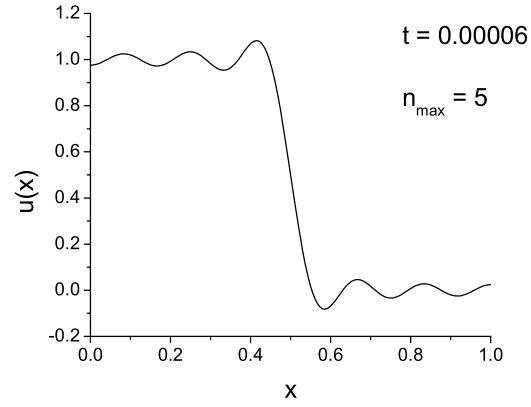
Figure 1: The $t = 0$ case.

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Figure 2: The $t = 0.00006$ case. At this time moment the cross-over from Gibbs-phenomenon behavior to a smooth behavior takes place at $n_{\max} \sim 25$.