Estimation of a diffusion constant in an equation with a dynamic boundary condition using Fourier analysis

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Abstract. In this paper, we derive a Fourier series expansion of the solution of a onedimensional diffusion equation with a dynamic boundary condition. Due to the boundary condition the spatial operator is *not self-adjoint* which makes the computation of the Fourier coefficients nonstandard. We use the first eigenfunction, i.e. the first term of the series, to estimate the diffusion constant of urea through a membrane.

Keywords: diffusion, dynamic boundary, Fourier series, parameter estimation

1 Introduction

To measure a diffusion constant of a given membrane with thickness L for a certain substance we use the following experiment: at one side of the membrane we put a donator of the substance in bulk. The corresponding concentration at this membrane site is assumed to be a constant u_D. At the other side, we place a finite reservoir with thickness K accepting the substance. The concentration $v(t)$ in the reservoir increases from 0 at $t = 0$ to u_D for $t \to \infty$. Let denote $u(t, x)$ the intra membrane concentration, i.e. the concentration of the substance in the membrane at distance x from the donator at time t. Then, by Fick's diffusion law, we obtain a system of a diffusion equation coupled with the reservoir concentration $v(t)$:

$$u_t = Du_{xx}, \quad x \in (0, L), \quad t \geq 0, \tag{1a}$$

$$u(t, 0) = u_D, \quad u(t, L) = v(t), \quad u(0, x) = 0, \tag{1b}$$

$$v'(t) = -\frac{D}{K}u_x(t, L), \quad v(0) = 0. \tag{1c}$$

The equation for the reservoir concentration $v(t)$ can be eliminated from the system. Differentiation of the boundary condition $u(t, L) = v(t)$ leads us to

$$u_t(t, L) = -\frac{D}{K}u_x(t, L). \tag{2}$$

If the diffusion equation is also valid at the boundary (i.e. if u_t and u_{xx} are continuous at $x = L$), we substitute (1c) by

$$u_{xx}(t, L) = -\frac{1}{K}u_x(t, L) \tag{3}$$

This dynamic boundary condition is a generalization of Dirichlet and Neumann conditions. For $K \to 0$, we see $u_x(t, L) \to 0$ (Eq. (2)) and for $K \to \infty$ we have $u(t, L) = 0$ (Eq. (3)). In both cases, analytic solutions

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in terms of Fourier series are well known, e.g. see [3]. In the following, we derive a similar series for the generalized problem (1a),(1b),(3) and use this series to estimate the diffusion constant D for an application from pharmacy. Note, that the diffusion system under consideration can also be interpreted in terms of heat conduction and thermal buffering.

Related to our work is the abstract existence theory in [6] for more general parabolic equations with dynamic boundary conditions. However, our specific case is not covered.

2 Separation-Ansatz

We seek a solution of the linear problem (1a),(1b),(3) using a separation ansatz. We start with a reduced problem with homogenized Dirichlet condition.

Lemma 1. *The solution $u(t,x)$ of the system*

$$u_t = u_{xx}, \quad x \in [0,1], \quad t \geq 0, \tag{4a}$$
$$u(0,x) = 1 \tag{4b}$$
$$u(t,0) = 0 \tag{4c}$$
$$\kappa u_{xx}(t,1) + u_x(t,1) = 0, \quad \kappa \geq 0 \tag{4d}$$

is almost everywhere given by the convergent Fourier series

$$u(t,x) = \sum_{n=0}^{\infty} c_n \exp(-\lambda_n^2 t) \sin \lambda_n x, \tag{5}$$

with eigenvalues $\lambda_n \in [n\pi, (n+1/2)\pi]$ defined by

$$\lambda_n \kappa \sin \lambda_n = \cos \lambda_n, \tag{6}$$

and

$$c_n = \frac{2}{\lambda_n \left(1 + \kappa \sin^2 \lambda_n\right)}. \tag{7}$$

Proof. Assuming that the variables are separable leads us immediately to an eigenvalue problem for a second order boundary value problem of the form

$$\phi_n''(x) = -\lambda_n^2 \phi_n(x) \tag{8a}$$
$$\phi_n(0) = 0 \tag{8b}$$
$$\kappa \phi_n''(1) + \phi_n'(1) = 0. \tag{8c}$$

From (8a) and (8b) follows $\phi_n(x) = c \sin \lambda_n x$. The eigenvalues λ_n can be computed (numerically) from the condition at the right boundary (8c), i.e.

$$\lambda_n \kappa \sin \lambda_n - \cos \lambda_n = 0. \tag{9}$$

A simple calculation gives $\lambda_n \kappa = \cot \lambda_n$. Since $\cot x$ has poles at $x = n\pi$ and is positive (but monotonously decreasing) for $x \in (n\pi, (n+\frac{1}{2})\pi)$, we have exactly one eigenvalue in each interval $\lambda_n \in [n\pi, (n+1/2)\pi]$. Now, we have the series (5) with eigenvalues (6). The parameters c_n have to be chosen to satisfy the initial condition (4b). But due to the dynamic boundary condition, the spatial operator $\frac{\partial^2}{\partial x^2}$ is *not self-adjoint* and hence the eigenfunctions $\sin \lambda_n x$ are not orthogonally with respect to the inner L^2-product $\langle \cdot, \cdot \rangle$. But we can use a different product $b(\phi, \psi) := \langle \phi, \psi \rangle + \kappa \phi(1)\psi(1)$. $b(\phi, \psi)$ is a bilinear form making the operator self-adjoint,

$$b(\phi_{xx}, \psi) - b(\phi, \psi_{xx}) = \phi_x \psi - \phi \psi_x|_1 + \kappa(\phi_{xx}\psi - \phi\psi_{xx}) = 0. \tag{10}$$

Since $\kappa \geq 0$ the bilinear form $b(\cdot,\cdot)$ is positive and hence a scalar product. The initial condition (4b) requires (almost everywhere)

$$1 = u(0,x) = \sum_{n=0}^{\infty} c_n \sin \lambda_n x, \quad x \in [0,1], \tag{11}$$

and, by application of $b(\sin \lambda_n x, \cdot)$ and use of the orthogonality (Eq. (10)), we have necessary

$$c_n = \frac{b(1, \sin \lambda_n x)}{b(\sin \lambda_n x, \sin \lambda_n x)} \tag{12}$$

We compute the integrals

$$b(1, \sin \lambda_n x) = \int_0^1 \sin \lambda_n x \, dx + \kappa \sin \lambda_n = -\frac{1}{\lambda_n}(\cos \lambda_n - 1) + \kappa \sin \lambda_n = \frac{1}{\lambda_n},$$
$$b(\sin \lambda_n x, \sin \lambda_n x) = \frac{\pi}{2} - \frac{1}{2}\int_0^1 \cos 2\lambda_n x \, dx + \kappa \sin^2 \lambda_n = \frac{1}{2}\left(\pi + \kappa \sin^2 \lambda_n\right),$$

and obtain (7). The convergence of the Fourier series can be studied in the norm induced by the bilinear form $b(\cdot,\cdot)$ $\|\phi\|_b := \sqrt{b(\phi,\phi)}$. Since $\lambda_n \geq n$ we have

$$\|\sum_{n=0}^{\infty} c_n \exp(-\lambda_n^2 t) \sin \lambda_n x\|_b^2 = \sum_{n=0}^{\infty} c_n^2 \exp(-2\lambda_n^2 t) \frac{1}{\lambda_n c_n} = \sum_{n=0}^{\infty} \exp(-2\lambda_n^2 t) \frac{2}{\lambda_n^2 (1 + \kappa \sin^2 \lambda_n)} < \infty.$$

Obviously, we have $\|u\|_2 \leq \|u\|_b$, i.e. the series converges also in L^2 norm.
It remains to show that Eq. (12) is sufficient to ensure (11), i.e., more generally, we have to show the completeness of the eigenfunction function system. For details, see next section 5. □

Remark 1. The boundary value system (8) is of Sturm-Liouville type (e.g. see [1, 2]). But (to the knowledge of the authors) the dynamic boundary condition (8c) has not been treated before within that context.

Remark 2. Let denote $H := H^1_{0,\cdot}[0,1]$ the Hilbert space of functions ϕ with $\phi(0) = 0$ and $[\phi, \psi] := \langle \phi', \psi' \rangle$ the corresponding dotproduct. A function $\phi \in H$ is a weak solution of (8) iff

$$\forall \psi \in H: \quad [\psi, \phi] + \lambda^2 b(\psi, \phi) = 0 \tag{13}$$

since

$$[\psi, \phi] + \lambda^2 b(\psi, \phi) = (\phi'(1) - \lambda\kappa\phi(1))\psi(1) - \int_0^1 (\phi'' + \lambda^2 \phi)\psi \, dx. \tag{14}$$

Since $b(\cdot,\cdot)$ is a compact symmetric operator on the separable Hilbert space H, the existence of a complete orthonormal system of eigenvectors follows from Hilbert-Schmidt Theory, see [7]. We thanks Ch. Grossmann for the fruitful discussion about the weak formulation.

Using the lemma, we can give a series for the original problem (1a),(1b),(3).

Theorem 1. *The system*

$$u_t = D u_{xx}, \quad x \in [0, L], \quad t \geq 0, \tag{15a}$$
$$u(0,x) = 0, \quad u(t,0) = u_D, \tag{15b}$$
$$K u_{xx}(t,L) + u_x(t,L) = 0 \tag{15c}$$

has a solution $u(t,x)$ given almost everywhere by a Fourier series

$$\frac{u(t,x)}{u_D} = 1 - \sum_{n=0}^{n} c_n \exp(-\lambda_n^2 D t / L^2) \sin(\lambda_n \frac{x}{L}), \tag{16}$$

with $\kappa = \frac{K}{L}$ and eigenvalues $\lambda_n \in [n\pi, (n+1/2)\pi]$ defined by

$$\lambda_n \kappa \sin \lambda_n = \cos \lambda_n, \tag{17}$$

and

$$c_n = \frac{2}{\lambda_n \left(1 + \kappa \sin^2 \lambda_n\right)}. \tag{18}$$

Proof. The substitutions $u \leftarrow 1 - u/u_D$, $x \leftarrow x/L$ and $t \leftarrow tD/L^2$ reduce the system (15) to the prerequisites of Lemma 1 and hence the theorem follows immediately. □

Remark 3. For $\kappa \to 0$ (i.e. Neumann BC) we have $\lambda_n \to (n+1/2)\pi$. Then the theorem above reproduces the well-known solution

$$\frac{u(t,x)}{u_D} = 1 - \frac{4}{\pi} \sum_{n=0}^{\infty} \frac{1}{2n+1} \exp\left(-\left[\frac{2n+1}{2}\pi\right]^2 Dt/L^2\right) \sin\left(\frac{2n+1}{2}\pi \frac{x}{L}\right). \tag{19}$$

□

Remark 4 (Direct numerical solution of the system (15)**).** To confirm our expansion we also computed a numerical solution of (15) using finite differences. Let $h = L/n$ and $x_i = ih$. We approximate $u(t, x_i)$ by $u_i^h(t)$, $i = 0, \dots, n$. Then, we obtain a linear ODE system for the grid values u_i^h

$$\frac{d}{dt} u^h(t) = M u^h(t), \quad u^h(0) = e_1 \in \mathbb{R}^{n+1},$$

with a matrix M given by

$$M = \frac{D}{h^2} \begin{pmatrix} 0 & 0 & 0 & \dots & & & \\ 1 & -2 & 1 & & & & \\ & \ddots & \ddots & \ddots & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & & 1 & -2 & 1 \\ & & & & & \alpha & -\alpha \end{pmatrix}. \quad \alpha = \frac{h}{K}$$

The exact solution of that semidiscrete system is given by $u(t, L) \approx u_n^h(t) = e_{n+1}^T \exp(Mt) e_1$. We computed the error $e(\kappa) := \|u(t,L) - u_n^h(t)\|_\infty$ for system (4) for different values of κ. We used $n = 20$ terms in the sum as well as $n = 20$ spatial discretization points. For $\kappa = 0.001, 0.01$, 0.1, 1, 10 and 1000 we have $e \approx 2.5 \cdot 10^{-2}$, $2.5 \cdot 10^{-2}$, $2 \cdot 10^{-2}$, $7 \cdot 10^{-3}$, $8 \cdot 10^{-4}$ and $8 \cdot 10^{-5}$. For larger values of t, the error tends to 0. □

3 Computation of the Fourier series

To take advantage of Fourier series representation (5) for the solution of the system (4) we just need numerical approximations to the eigenvalues λ_n. Using the expansions

$$(-1)^n \sin(n\pi + h) \approx h, \quad (-1)^n \cos(n\pi + h) \approx 1 - \frac{h^2}{2}, \quad \lambda_n = n\pi + h, \quad h \to 0$$

we obtain from (6) an approximation formula

$$\lambda_n \approx \lambda_n^0 := \frac{n\pi + \kappa n\pi + \sqrt{2 + 4\kappa + \kappa^2 n^2 \pi^2}}{2\kappa + 1}, \tag{20}$$

which preserves the enclosing interval $n\pi < \lambda_n^0 < (n+1/2)\pi$ and is asymptotically exact for large κ, i.e. $\lambda_n^0 \to n\pi$ for $\kappa \to \infty$. Eq. (20) be used as a predictor for a Newton iteration of the form

$$\lambda_n = \lim_{l\to\infty} \lambda_n^l, \quad \text{with} \quad \lambda_n^{l+1} = \phi(\lambda_n^l), \quad \text{where} \quad \phi(\lambda) = \lambda - \frac{\kappa\lambda\sin\lambda - \cos\lambda}{\kappa\lambda\cos\lambda + \sin\lambda + \kappa\sin\lambda}. \tag{21}$$

Both, the predictor and the Newton iteration, can be easily implemented within a computer algebra system like Mathematica. For reference, we include our code here which computes the first 20 terms of the solution of the system (4) for a fixed κ.

```
(* Computation of the Fourier series (Eq. (5)) in Mathematica
   u[kappa] is the an expression containing the variables x and t *)
u[kappa_] := Module[{predictor, lambda, coeff, newtonstp},
  predictor[n_] = l /. Solve[l kappa(l-n Pi)-(1-(l - n Pi)^2/2)==0,l][[2]];
  f             = l kappa Sin[l]-Cos[l];
  newtonstp[l_] = N[l-f/D[f,l],20];
  lambda[n_]   := FixedPoint[newtonstp, predictor[n]];
  coeff[n_]    := 2 Sin[lambda[n x]]/(lambda[n](1+kappa Sin[lambda[n]]^2));
  Sum[coeff[n] Exp[-lambda[n]^2 t], {n, 0, 20}]]
```

4 Estimation of the diffusion constant

Except for a short initial phase the solution of diffusion equation (15) is dominated by the eigenfunction $c_0 \exp(-\lambda_0 t D/L^2) \sin\lambda_0 x$ of the smallest eigenvalue λ_0. It is therefore obvious to design a simple approximation formula (which can be used comfortably for parameter fitting) based on that first eigenfunction. We use the predictor Eq. (20), i.e. $\lambda_0^0 \approx 1/\sqrt{\kappa + 1/2}$, and $c_0 \approx 1$ and obtain the model for the solution of the system (15)

$$u(t, L) \approx u_D \cdot \left(1 - \exp\left(-\frac{Dt}{KL + 1/2L^2}\right)\right) \tag{22}$$

Note, that after a scaling $t \to Dt/L^2$ the model (22) as well as the Fourier series (16) depend only on one parameter, namely $\kappa = K/L$. Hence, to study the error of the approximation (22) compared with the exact solution $u(t, L)$ it is sufficient to vary κ only. Without loss of generality we can set $D = L = u_D = 1$. The plot in Fig. 1 comparing the series (16) with the simple approximation (22) above shows a good qualitative agreement for $\kappa = 0.1, 1, 5, 20$, particularly for $\kappa = 5$ and $\kappa = 20$.

Artificial membranes are often used to study diffusion processes and to estimate the rate of penetration of drugs into the outermost layer of the skin, the *stratum corneum*. Such membranes are more homogeneous than skin and data analysis is simplified. In this work, the diffusion of water from 20 % (w/w) aqueous urea solution has been investigated. Polydimethylsiloxane (PDMS) membranes containing 12.5 % (w/w) polyethylene glycol 400 (PEG 400) were used. Membrane thickness was $L = 78\mu\text{m}$ and the reservoir height $K = 550\mu\text{m}$, i.e. $\kappa = 7.051$. Fourier transform infrared - attenuated total reflectance (FTIR-ATR) spectroscopy coupled with a diffusion cell has been used to examine the diffusion of water through the membrane (e.g. see [4]). The concentration of water in the acceptor compartment was measured at the bottom of the reservoir on the PEG/zinc-selenide crystal interface. The receptor compartment contained 550 μl PEG. 3 ml of aqueous urea solution was applied as donor solution on top of the membrane. The appearance of water peak during the course of penetration was detected and the area under peak integrated. An increase in concentration of water in the acceptor compartment with time was observed. It was assumed that peak area and concentration are proportional. A typical data set is shown in Fig.2.

Using the series (16) and nonlinear least-squares approximation we obtain $D = 2415.54\mu\text{m}^2\text{min}^{-1}$. Based on (22), we find a best-approximation with $D = 2387.67\mu\text{m}^2\text{min}^{-1}$. Since this small ($\approx 1\%$) error of using the formula (22) instead of the series (16) is much smaller then the accuracy of the measurement method we conclude that for our application a curve fitting based on (22) is quite adequate.

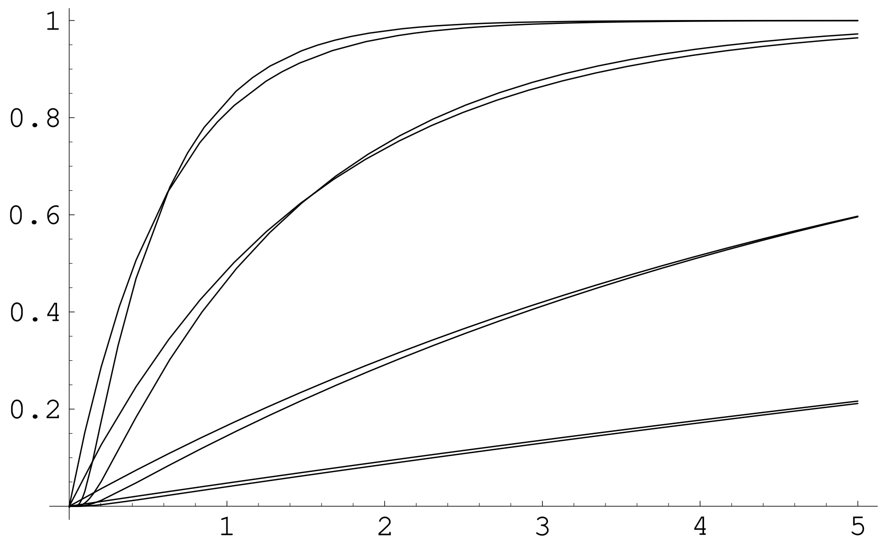

Figure 1: A comparison of the Fourier series (16) and the simple model (22) based on the first eigenfunction only for $\kappa = 0.1, 1, 5, 20$ (curves pairs from left to right). An obvious distinction between the series and the simple model is possible for $t = 0$. The exact solution has slope 0 but the approximation has slope $1/\sqrt{\kappa + 1/2}$.

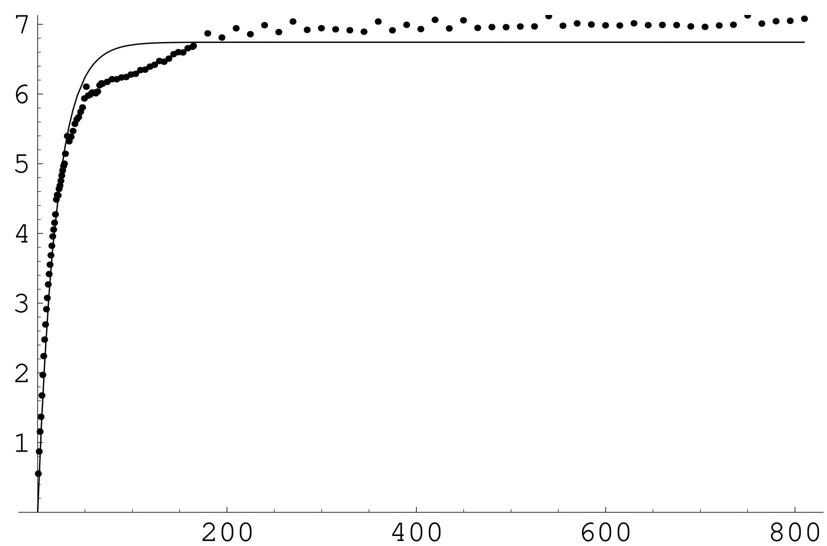

Figure 2: Diffusion of water through a PEG/PDMS membrane. Area of water OH-stretch band versus time. The fitted curve with $D = 2387.67 \mu\mathrm{m}^2 \mathrm{min}^{-1}$ was obtained using the model (22).

5 A conjecture on the completeness of the eigenfunction system

There is no general recipe to prove completeness of a system of functions. Profound theorems like the Stone-Weierstraß Theorem are powerful tools in proving completeness of the system of polynoms or the system of trigonometric functions. Unfortunately, we have not found a general theorem that covers our problem.
We tackle the problem by a careful examination of Greens function. Our strategy is based on the ideas used in [5] to prove completeness of the eigenfunctions of self-adjoint second order differential equations.

Conjecture 1. *For each* $\kappa > 0$ *the system of functions* $\sin \lambda_n x$. $n = 1, \dots$ *where* λ_n *is given by* (6) *is complete in* L^2.

In the remainder of this section we will present our ideas how to prove that conjecture. The (until now) missing detail is the very technical estimation of asymtotic bounds for Greens function.

1. We construct the special solution of $u'' + \mu u = g(x)$ under the given boundary conditions.
2. The solution exists if μ is not an eigenvalue of $-\frac{d^2}{dx^2}$. It can be given in terms of Greens function
$$u(x, \mu) = \int_0^1 G(x, \xi, \mu) g(\xi) d\xi + H(x, \lambda) g(1).$$
3. Greens function is investigated for $\mu \in \mathbb{C}$. It has simple poles in the eigenvalues $\mu = \mu_k := \lambda_k^2$.
4. By means of the residue theorem we can express Greens function as a series
$$G(x, \xi, \mu) = \sum_{k=0}^{\infty} \frac{1}{\mu - \mu_k} \phi_i(x) \phi_i(\xi) \tag{23}$$
$$H(x, \mu) = \sum_{k=0}^{\infty} \frac{\kappa}{\mu - \mu_k} \phi_i(x) \phi_i(1) \tag{24}$$
where ϕ_i are the normalized eigenfunctions.
5. We consider the equation $u'' = f''$ with solution $u = f$, and express f by Greens function – the result is the Fourier series.

5.1 Construction of the special solution, step 1 and 2.

The solutions of the homogenous equation $u'' + \mu u$ are spanned by the two fundamental solutions
$$\begin{aligned} y_1(x, \mu) =& \frac{\sin \sqrt{\mu} x}{\sqrt{\mu}}, y_1(0, \mu) = 0, y_1'(0, \mu) = 1 \\ y_2(x, \mu) =& \frac{\sin \sqrt{\mu}(x-1)}{\sqrt{\mu}}, y_2(1, \mu) = 0, y_2'(1, \mu) = 1. \end{aligned}$$
We combine both to obtain the solution of the inhomogenous problem by the variation of constants. Note, that we skip all arguments μ. The ansatz $y(x) = k_1(x) y_1(x) + k_2(x) y_2(x)$ leads to the system
$$\begin{pmatrix} y_1(x) & y_2(x) \\ y_1'(x) & y_2'(x) \end{pmatrix} \begin{pmatrix} k_1'(x) \\ k_2'(x) \end{pmatrix} = \begin{pmatrix} 0 \\ g(x) \end{pmatrix} \text{ with solution}$$
$$\begin{aligned} k_1'(x) =& -\frac{y_2(x)}{D(x)} g(x) \\ k_2'(x) =& \frac{y_1(x)}{D(x)} g(x) \text{ where} \\ D(x) =& y_1(x) y_2'(x) - y_1'(x) y_2(x) = \frac{\sin \sqrt{\mu} x}{\sqrt{\mu}}. \end{aligned}$$

The solution $y(x)$ has to satisfy the boundary conditions. The homogenous Dirichlet condition at $x = 0$ is equivalent to $k_2(0) = 0$. This is guaranteed by the ansatz

$$k_1(x) = \int_x^1 \frac{y_2(\xi)}{D} g(\xi) d\xi + c_1 \qquad\qquad k_2(x) = \int_0^x \frac{y_1(\xi)}{D} g(\xi) d\xi.$$

We insert the ansatz into the second boundary condition $y'(1) + \kappa y''(1) = 0$ and obtain

$$\begin{aligned} 0 =& k_1'(1)y_1(1) + k_2'(1)y_2(1) + k_1(1)y_1'(1) + k_2(1)y_2'(1) + \\ & \kappa(k_1''(1)y_1(1) + k_2''(1)y_2(1) + 2(k_1'(1)y_1'(1) + k_2'(1)y_2'(1)) + k_1(1)y_1''(1) + k_2(1)y_2''(1)) \\ =& 0 + c_1 y_1'(1) + k_2(1) + \kappa\left(-\frac{y_2'(1)}{D(1)} g(1) + 2g(1) + c_1 y_1''(1)\right) \\ c_1 =& -\frac{1}{\cos\sqrt{\mu} - \kappa\sqrt{\mu}\sin\sqrt{\mu}}\left(\int_0^1 \frac{y_1(\xi)}{D} g(\xi) d\xi + \kappa g(1)\right) \end{aligned}$$

Putting all together we obtain the solution

$$\begin{aligned} y(x,\mu) =& \int_0^x \frac{\sin\sqrt{\mu}\xi}{\sqrt{\mu}}\left(\sin\sqrt{\mu}(x-1) - \frac{y_1(x)}{\cos\sqrt{\mu} - \kappa\sqrt{\mu}\sin\sqrt{\mu}}\right) g(\xi) d\xi \\ &+ \int_x^1 \frac{\sin\sqrt{\mu}x}{\sqrt{\mu}}\left(\sin\sqrt{\mu}(\xi-1) - \frac{y_1(\xi)}{\cos\sqrt{\mu} - \kappa\sqrt{\mu}\sin\sqrt{\mu}}\right) g(\xi) d\xi \\ &- \frac{\kappa y_1(x)}{\cos\sqrt{\mu} - \kappa\sqrt{\mu}\sin\sqrt{\mu}} g(1). \end{aligned} \tag{25}$$

The representation with Greens functions G, H follows directly from here.

5.2 Singularities in Greens function, step 3

Greens functions G, H have poles exactly at the points $\mu = \lambda_k^2$, $k = 0, \ldots$. An expansion of the denominator at these points gives

$$\begin{aligned} \cos\sqrt{\mu} - \kappa\sqrt{\mu}\sin\sqrt{\mu} =& 0 - ((1+\kappa)\sin\lambda_k + \kappa\lambda_k\cos\lambda_k)(\sqrt{\mu} - \lambda_k) + \mathcal{O}\left((\sqrt{\mu} - \lambda_k)^2\right) \\ =& -(1 + \kappa + \kappa^2\lambda_k^2)\sin\lambda_k \frac{1}{2\lambda_k}(\mu - \lambda_k^2) + \mathcal{O}\left((\mu - \lambda_k^2)^2\right). \end{aligned}$$

It is easily verified that all poles are of order one. By the residue theorem we write Greens function as a contour integral

$$G(x,\xi,\mu) = \sum_{k=0}^{N} \frac{a_k}{\mu - \lambda_k^2} + \int_{\Gamma_N} \frac{G(x,\xi,\zeta)}{\zeta - \mu} d\zeta \tag{26}$$

$$H(x,\mu) = \sum_{k=0}^{N} \frac{b_k}{\mu - \lambda_k^2} + \int_{\Gamma_N} \frac{H(x,\xi,\zeta)}{\zeta - \mu} d\zeta \tag{27}$$

where the contours Γ_N are choosen such that exactly the eigenvalues $\lambda_0, \ldots, \lambda_N$ are inside of the contour Γ and the residues a_k, b_k are the coefficients of the $(\mu - \lambda_k^2)^{-1}$-term in the Laurent expansion. A short calculation gives the residues

$$\begin{aligned} a_k =& \frac{\sin\lambda_k x \sin\lambda_k\xi}{\frac{1}{2}(1 + \kappa\sin^2\lambda_k)} = \phi_k(x)\phi_k(\xi) \\ b_k =& \kappa\frac{\sin\lambda_k x \sin\lambda_k}{\frac{1}{2}(1 + \kappa\sin\lambda_k^2)} = \kappa\phi_k(x)\phi_k(1). \end{aligned}$$

The functions ϕ_k are the eigenfunctions normalized with respect to the norm induced by the inner product $b(\cdot,\cdot)$.

5.3 Asymptotic beheaviour of Greens function – point 4.

It remains to show that a sequence of contours Γ_N can be chosen such that the integrals in (26) and (27) tend to zero. To this end it suffices to show that G, H are bounded for suitable contours by

$$G(x,\xi,\mu) \leq \frac{M}{\sqrt{|\mu|}}$$
$$H(x,\mu) \leq \frac{M}{\sqrt{|\mu|}}.$$

This is the crucial point where we have not succeeded yet, we hope to accomplish in further work.

5.4 Final step

Let f be an arbitary function, twice differentiable, satisfying the boundary conditions. For $\mu = 0$ we have f satisfying the differential equation with inhomogenity $g(x) = f''(x)$. We express f by Greens function

$$f(x) = \int_0^1 \sum_{k=0}^{\infty} -\frac{1}{\mu_k}\phi_k(x)\phi_k(\xi)f''(\xi)d\xi + \sum_{k=0}^{\infty} -\frac{\kappa}{\mu_k}\phi_k(x)\phi_k(1)f''(1) \tag{28}$$

We exchange integration and summation because the series converges uniformly with respect to x and ξ. Further, the operator $\frac{\partial^2}{\partial x^2}$ is selfadjoint with respect to the bilinear form $b(\cdot,\cdot)$. We end with

$$f(x) = \sum_{k=0}^{\infty} -\frac{1}{\mu_k}\phi_k(x)b(\phi_k, f'') = \sum_{k=0}^{\infty} -\frac{1}{\mu_k}\phi_k(x)b(\phi_k'', f) \tag{29}$$
$$= \sum_{k=0}^{\infty} \phi_k(x)b(\phi_k, f) \tag{30}$$

This proves that every twice continiously differentiable function that satisfies the boundary conditions can be expressed by an uniformly convergent Fourier series in the eigenfunctions. From that we conclude that the linear space generated by the eigenfunctions lies dense in L^2.

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