MMP I
Solution Sheet 11

HS 21
Prof. Ph. Jetzer

L. Buonocore, M. Loechner, X. Liu, M. Ebersold
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Exercise 1 [Schrödinger equation (6 points)]

$u''(x) + [\lambda - W(x)]u(x) = 0$ with $u(\pm\infty) = 0$

Potential $W = \begin{cases} 0 & \text{for } |x| \geq a \\ -\frac{K}{2a} & \text{for } |x| < a \end{cases}$

$K > 0$, $a > 0$

Notice that $W(x) = W(-x)$ (even) $\rightarrow$ this implies that if $u(x)$ is a solution $\rightarrow u(x) = u(-x)$

a) let's consider 3 regions

- $\underline{x \leq -a}$
  $W(x) = 0$
  $\begin{cases} u'' + \lambda u = 0 \\ u(-\infty) = 0 \end{cases}$
  if $\lambda > 0$: $u(x) = A\cos(\sqrt{\lambda}x) + B\sin(\sqrt{\lambda}x)$
  $\lim\limits_{x\to-\infty} u(x) \rightarrow$ it doesn't exist $\neq 0$. No solution for $\lambda > 0$
  if $\lambda < 0$: $u(x) = Ae^{\sqrt{-\lambda}x} + Be^{-\sqrt{-\lambda}x}$
  $\lim\limits_{x\to-\infty} u(x) = 0 \leftrightarrow B = 0$
  $\Rightarrow$ The solution for $x \leq -a$ is $u(x) = Ae^{\sqrt{-\lambda}x}$ with $\lambda < 0$
- $\underline{x \geq a} \rightarrow$ the symmetry of the problem tells us that the solution is $u(x) = Ae^{-\sqrt{-\lambda}x}$ with $\lambda < 0$
- $\underline{-a < x < a}$:
  $u'' + (\lambda + \frac{K}{2a})u = 0$
  let's define $\alpha^2 = \lambda + \frac{K}{2a} \rightarrow u'' + \alpha^2 u = 0$

$\rightarrow$ if $\alpha^2 > 0$:

$\lambda > -\frac{K}{2a}$

$u(x) = C\cos(\alpha x) + D\sin(\alpha x)$

$u(x) = u(-x) \rightarrow D = 0$

$\rightarrow$ the solution for $|x| < a$ with $\alpha^2 > 0$ is $u(x) = C\cos(\alpha x)$ with $\alpha^2 = \lambda + \frac{K}{2a}$

$\rightarrow$ if $\alpha^2 < 0 \leftrightarrow \lambda < -\frac{K}{2a} < 0$

$u(x) = Ce^{\sqrt{-\alpha^2}x} + De^{-\sqrt{-\alpha^2}x}$

$u(x) = u(-x) \rightarrow Ce^{\sqrt{-\alpha^2}x} + De^{-\sqrt{-\alpha^2}x} = Ce^{-\sqrt{-\alpha^2}x} + De^{\sqrt{-\alpha^2}x}$

$\rightarrow C = D$

$u(x) = C(e^{\sqrt{-\alpha^2}x} + e^{-\sqrt{-\alpha^2}x}) = 2C\cosh(\sqrt{-\alpha^2}x)$ with $\lambda < -\frac{K}{2a} < 0$

$\rightarrow$ if $\alpha^2 = 0 \leftrightarrow \lambda = -\frac{K}{2a}$

$u''(x) = 0 \overset{\int dx}{\rightarrow} u'(x) = A \overset{\int dx}{\rightarrow} u(x) = Ax + B \Rightarrow u(x) \neq u(-x) \lightning$ no solution

$$\text{so: } \begin{cases} |x| \geq a & u(x) = Ae^{-\sqrt{-\lambda}|x|} \quad (\lambda < 0) \\ |x| < a & \begin{cases} \lambda > -\frac{K}{2a} & u(x) = C\cos(\alpha x) \\ \lambda < -\frac{K}{2a} & u(x) = 2C\cosh(\sqrt{-\alpha^2}x) \end{cases} \end{cases}$$

Continuity of $u(x)$ and $u'(x)$ in $x = \pm a$:

- $\underline{x = a}$
  - $\underline{\alpha^2 > 0}$, $\lambda > -\frac{K}{2a}$

    $u(a) \Rightarrow C\cos(\alpha a) = Ae^{-\sqrt{-\lambda}a}$

    $u'(x) \Rightarrow -\alpha C\sin(\alpha x) = -\sqrt{-\lambda}Ae^{-\sqrt{-\lambda}a}$

    $-\frac{u'(a)}{u(a)} \rightarrow \alpha\tan(\alpha a) = \sqrt{-\lambda} = \sqrt{\lambda + \frac{K}{2a}}\tan\left(\sqrt{\lambda + \frac{K}{2a}}a\right)$ for $-\frac{K}{2a} < \lambda < 0$

    $\lambda_1^{(a)} = \min\left\{\lambda | \sqrt{-\lambda} = \alpha\tan(\alpha a) \text{ with } \alpha^2 = \lambda + \frac{K}{2a}\right\}$
  - $\underline{a^2 < 0}$, $\lambda < -\frac{K}{2a}$

    $u(-a) \rightarrow 2C\cosh(\sqrt{-\alpha^2}a) = Ae^{-\sqrt{-\lambda}a}$

    $u'(-a) \rightarrow \sqrt{-\alpha^2}2C\sinh(\sqrt{-\alpha^2}a) = -A\sqrt{-\lambda}e^{-\sqrt{-\lambda}a}$

    $\underbrace{\sqrt{-\alpha^2}\tanh(\sqrt{-\alpha^2}a)}_{>0} = \underbrace{-\sqrt{-\lambda}}_{<0}$

    No Solution.
- $\underline{x = -a}$
  - $\underline{\alpha^2 > 0}$

    $u(-a) \rightarrow C\cos(\alpha a) = Ae^{-\sqrt{-\lambda}a}$

    $u'(-a) \rightarrow \alpha C\sin(\alpha a) = \sqrt{-\lambda}e^{\sqrt{-\lambda}a}$

    $\alpha\tan(\alpha a) = \sqrt{-\lambda}$

    $\lambda_1^{(a)} = \min\left\{\lambda | \sqrt{-\lambda} = \alpha\tan(\alpha a) \text{ with } \alpha^2 = \lambda + \frac{K}{2a}\right\}$

- $\underline{\alpha^2 < 0}$, $\lambda < -\frac{K}{2a}$
  $u(-a) \to +2C\cosh(\sqrt{(-\alpha^2)}a) = Ae^{\sqrt{-\lambda}a}$
  $u'(-a) \to -\sqrt{-\alpha^2}2C\sinh(\sqrt{-\alpha^2}a) = \sqrt{-\lambda}Ae^{\sqrt{-\lambda}a}$
  $-\underbrace{\sqrt{-\alpha^2}}_{>0}\underbrace{\tanh(\sqrt{-\alpha^2}a)}_{>0} = \underbrace{\sqrt{-\lambda}}_{>0}$
  No solution.

$\to \lambda_1^{(\pm a)} = \min\left\{\lambda | \sqrt{-\lambda} = \alpha\tan(\alpha a) \text{ with } \alpha^2 = \lambda + \frac{K}{2a}\right\}$

b) Rayleigh Principle:

$\lambda_{min} \leq R(u)$, $\lambda_{min} = R(u_{\lambda_{min}})$, $u_{\lambda_{min}}$ = corresponding eigenfunction

$u'' + (\lambda - W)u = 0$

$-u'' + W(u) = \lambda u \to H = -\frac{\partial^2}{\partial x^2} + W$

Rayleigh quotient $R_{(u)}^{(a)} = \frac{(Hu,u)}{u,u} = \frac{\int\limits_{-\infty}^{\infty}(-u''+Wu)\overline{u}dx}{\int\limits_{-\infty}^{\infty}u^2dx} = \frac{\int\limits_{-\infty}^{\infty}-u''\overline{u}dx + \int\limits_{-a}^{a}-\frac{K}{2a}u^2dx}{\int\limits_{-\infty}^{\infty}u^2dx}$

$(u'\overline{u})' = u''\overline{u} + u'\overline{u}' = u''\overline{u} + |u'|^2$, $u'\overline{u}|_{-\infty}^{\infty} = 0$, $u(x) \in \mathbb{R}$

$$\frac{\int\limits_{-\infty}^{\infty}-u''\overline{u}dx + \int\limits_{-a}^{a}-\frac{K}{2a}u^2dx}{\int\limits_{-\infty}^{\infty}u^2dx} = \frac{\int\limits_{-\infty}^{\infty}u'^2dx - u'\overline{u}|_{-\infty}^{\infty} - \int\limits_{-a}^{a}\frac{K}{2a}u^2dx}{\int\limits_{-\infty}^{\infty}u^2dx} = \frac{\int\limits_{-\infty}^{\infty}u'^2dx - \int\limits_{-a}^{a}\frac{K}{2a}u^2dx}{\int\limits_{-\infty}^{\infty}u^2dx}$$

$$\Rightarrow R_{(u)}^{(a)} = \frac{\int\limits_{-\infty}^{\infty}u'^2dx - \int\limits_{-a}^{a}\frac{K}{2a}u^2dx}{\int\limits_{-\infty}^{\infty}u^2dx} \geq \lambda_1^{(a)}$$

We want to show that if $a < a^+ \to \lambda_1^{(a)} \leq \lambda_1^{(a^+)}$

for $0 < x < a$ $u \sim \cos(\alpha x)$

$|x| > a$ $u(x) \sim e^{-\sqrt{-\lambda}x}$

$\lambda \in (-\frac{K}{2a}, 0) \Rightarrow \alpha = \sqrt{\lambda + \frac{K}{2a}} \in (0, \frac{K}{2a})$. Since $\sqrt{-\lambda}$ is finite $\forall\lambda$ and $\alpha\tan(\alpha a) \overset{\alpha a \to \frac{\pi}{2}}{\longrightarrow} \infty$, $\alpha a < \frac{\pi}{2}$ for the lowest eigenvalue $\lambda_1^{(a)}$. Therefore its eigenfunction $u_1^{(a)} \sim \cos(\alpha(\lambda_1^{(a)})a) > 0$ and decreasing $\forall x \in [0, a]$ and thus satisfies these properties on the entire real line.

Notice that if $f(x) > 0$ and decreasing: $\frac{1}{L}\int\limits_0^L f^2(x)dx \leq \frac{1}{l}\int\limits_0^l f^2(x)dx$ if $L \geq l$

Let's call $u_1^{(a^+)}$ the eigenfunction corresponding to $\lambda_1^{(a^+)}$

$$\lambda_1^{(a)} = R^{(a)}(u_1^{(a)}) \leq R^{(a)}(u_1^{(a^+)}) = \frac{\int\limits_{-\infty}^{\infty}(u_1^{(a^+)})'^2dx - \int\limits_{-a}^{a}\frac{K}{2a}(u_1^{(a^+)})^2dx}{\int\limits_{-\infty}^{\infty}u^2dx} = \frac{\int\limits_{-\infty}^{\infty}(u_1^{(a^+)})'^2dx - \frac{K}{a}\int\limits_0^a(u_1^{(a^+)})^2dx}{\int\limits_{-\infty}^{\infty}u^2dx}$$

For $a^+ > a$:

$$\frac{\int\limits_{-\infty}^{\infty}(u_1^{(a^+)})'^2dx - \frac{K}{a}\int\limits_0^a (u_1^{(a^+)})^2dx}{\int\limits_{-\infty}^{\infty} u^2dx} \leq \frac{\int\limits_{-\infty}^{\infty}(u_1^{(a^+)})'^2dx - \frac{K}{a^+}\int\limits_0^{a^+} (u_1^{(a+)})^2dx}{\int\limits_{-\infty}^{\infty} u^2dx} = R^{(a^+)}(u_1^{(a^+)}) = \lambda_1^{(a^+)}$$

$\lambda_1^{(a)} < \lambda_1^{(a^+)}$

Exercise 2 [Homogeneous string (6 points)]

a) We have to extremise $S[f]$ subject to the constraint $\int_0^1 (f(x))^2\,dx = 1$. Introducing a Lagrange multiplier λ we have

$$L = \int_0^1 \left(f'(x)\right)^2 dx - \lambda \int_0^1 (f(x))^2\,dx = \int_0^1 \left[\left(f'(x)\right)^2 - \lambda\,(f(x))^2\right] dx$$

Lets compute the variation of L to find the natural constraint:

$$\begin{aligned}
\delta L &= \delta\left[\int_0^1 \left(f'^2 - \lambda f^2\right) dx\right] = 2\int_0^1 f'\delta f' dx - 2\lambda \int f\delta f dx \\
&\underbrace{=}_{\delta f' = (\delta f)'} 2\int_0^1 f'(\delta f)' dx - 2\lambda\int_0^1 f\delta f dx \\
&= 2\left[f'\delta f\right]_0^1 - 2\int_0^1 f''\delta f dx - 2\lambda \int_0^1 f\delta f dx \\
&= 2\left[\underbrace{f'(1)}_{(*)}\delta f(1) - \cancel{f'(0)\underbrace{\delta f(0)}_{=0}}\right] \underbrace{- 2\int_0^1 \left(f'' + \lambda f\right)\delta f dx}_{(**)} = 0
\end{aligned}$$

$(**)$ is equivalent to the Euler-Lagrange equation.

$\rightarrow (*)$ must be 0 in order to have $\delta L = 0 \rightarrow$ natural constraint: $\underline{f'(1) = 0}$

b) $\delta L = 0 \rightarrow$ Euler-Lagrange equation:

$$\frac{\partial F}{\partial f} - \frac{d}{dx}\left(\frac{\partial F}{\partial f'}\right) = 0 \rightarrow \frac{d}{dx}\left(F - f'\frac{\partial F}{\partial f'}\right) = 0$$

$$\begin{aligned}
F = f'^2 - \lambda f^2 \rightarrow &\frac{d}{dx}\left(f'^2 - \lambda f^2 - f'2f'\right) = 0 \\
&-\frac{d}{dx}\left(f'^2 - \lambda f^2\right) = 0 \\
&-\cancel{2f'}f'' - \lambda\cancel{2f'}f = 0 \rightarrow -f'' = \lambda f \\
&\rightarrow \underline{-\frac{d^2}{dx^2}f(x) = \lambda f(x)}
\end{aligned}$$

$\rightarrow$ Eigenvalue problem for $A = -\frac{d^2}{dx^2}$ with $f(0) = 0$ and the natural constraint $f'(1) = 0$.
Is $Af = -\frac{d^2}{dx^2}f = \lambda f$ equivalent to $R[f] = \frac{(Af,f)}{(f,f)}$?

$$(Af,f) = -\int_0^1 f''(x)f(x)dx = \underbrace{-ff'\big|_0^1}_{-f(1)\cancel{f'(1)}+\cancel{f(0)}f'(0)=0} + \int_0^1 \left[f'(x)\right]^2 dx = \int_0^1 \left(f'(x)\right)^2 dx$$

$\rightarrow$ Yes, they are equivalent.

c) For $g_1 = x$:

$$R[g_1] = \frac{\int_0^1 dx}{\int_0^1 x^2 dx} = \frac{1}{\left[\frac{1}{3}x^3\right]_0^1} = 3$$

For $g_2 = -\frac{x^3}{6} + \frac{x}{2}$:

$$R[g_2] = \frac{\int_0^1 \left(-\frac{x^2}{2} + \frac{1}{2}\right)^2 dx}{\int_0^1 \left(-\frac{x^3}{6} + \frac{x}{2}\right) dx} = \frac{\left[\frac{x}{60}\left(3x^4 - 10x^2 + 15\right)\right]_0^1}{\left[x^3\left(\frac{x^4}{252} - \frac{x^2}{30} + \frac{1}{12}\right)\right]_0^1} = \frac{\frac{3-10+15}{60}}{\frac{5-42+105}{1260}} = \frac{\cancel{8}^{2}\ \cancel{1260}^{21}}{\cancel{60}_{1}\ \cancel{68}_{17}} = \frac{42}{17} \approx 2.4706$$

For $g_3 = \frac{x^5}{120} - \frac{x^3}{12} + \frac{5}{24}x$:

$$\begin{aligned} R[g_3] &= \frac{\int_0^1 \left(\frac{x^4}{24} - \frac{x^2}{4} + \frac{5}{24}\right)^2 dx}{\int_0^1 \frac{1}{120^2}\left(x^5 - 10x^3 + 25x\right)^2 dx} \\ &= \frac{\frac{1}{24^2}\left[\frac{x^9}{9} - \frac{12}{7}x^7 + \frac{46}{5}x^5 - 20x^3 + 25\right]}{\frac{1}{12^2}\left[\frac{x^{11}}{11} - \frac{20}{9}x^9 + \frac{150}{7}x^7 - 100x^5 + \frac{625}{3}x^3\right]} = \frac{1705}{691} \approx 2.4674 \end{aligned}$$

An upper bound for the lowest eigenvalue is $\lambda_{min} \leq R[g_3] \approx 2.4674$.

d) The resulting Euler-Lagrange equation is

$$f'' + \lambda f = 0$$

The general solution is given by

$$f(x) = a\sin(\sqrt{\lambda}x) + b\cos(\sqrt{\lambda}x)$$

Using the boundary condition $f(0) = 0$ we find $b = 0$. By applying the constraint $f'(1) = 0$ we have:

$$\begin{aligned} &a\cos(\sqrt{\lambda})\sqrt{\lambda} = 0 \text{ for } a \neq 0 \text{ and } \lambda \neq 0 \text{ (otherwise } f(x) = 0) \\ &\rightarrow \cos(\sqrt{\lambda}) = 0 \rightarrow \underline{\sqrt{\lambda} = (2n+1)\frac{\pi}{2} \text{ with } n \in \mathbb{Z}} \end{aligned}$$

$$\underline{\rightarrow \lambda_n = (2n+1)^2\frac{\pi^2}{4}, \quad f_n(x) = a_n \sin((2n+1)\frac{\pi}{2}x)}$$

and a_n can be determined using $\int_0^1 f_n(x)dx = 1$.

The first eigenvalue (i.e. the minimum) is $\underline{\lambda_0 = \frac{\pi^2}{4} \approx 2.4673 < R[g_3]}$

Notice that $g_1, g_2, g_3, ...$ become closer and closer to the series development of the sine function (which is the eigenfunction):

$$\sin x = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} x^{2n+1} = x - \frac{x^3}{3!} + \frac{x^5}{5!} ...$$

That's why $R[g_n]$ becomes closer to λ_0 as n grows.