see any ODE book.

References: • Freiling/Yurko "Inverse Sturm-Liouville problems and their Applications"

Schrödinger ODEs

Consider the ODE $-u'' + q(x)u = f(x)$
with initial conditions $u(x_0) = u_0$, $u'(x_0) = u_0'$
We have seen that this problem can be written as

(*) $$u(x) - \int_{x_0}^{x} q(y)(x-y)\,u(y)\,dy = u_0 + u_0'(x-x_0) - \int_{y}^{x} f(y)(x-y)\,dy$$
$$=: F(x)$$

If $q \in L^2([a,b])$ and $f \in L^2([a,b])$, then we have seen from the theory of Volterra integral equations that (*) has a unique solution in $L^2([a,b])$. In fact, this solution is absolutely continuous because $q(y)u(y)$ and $f(y)$ are locally integrable.

Define the differential operator $L = -\frac{d^2}{dx^2} + q(x)$
so that $Lu = -u'' + q(x)u$.

On an interval $[a,b]$, let $\langle u,v\rangle = \int_a^b u\bar{v}$ be the L^2-inner product. The calculation

$$\langle Lu,v\rangle - \langle u,Lv\rangle = \int_a^b (u\bar{v}'' - \bar{v}u'') = \int_a^b (u\bar{v}' - \bar{v}u')'$$
$$= \int_a^b \frac{d}{dx} W(u,\bar{v})\,dx = W(u,\bar{v})\Big|_a^b$$

shows that L is not symmetric because of the boundary values of the Wronskian $(u\bar{v}' - \bar{v}u')$ of u and $\bar{v}$. The domain of L requires careful restriction to obtain a good spectral theory.

If $Lu = \lambda u$ and $Lv = \bar{\lambda} v$, then $\langle Lu, v\rangle = \lambda \langle u, v\rangle = \langle u, Lv\rangle$, so the Wronskian $W(u, \bar{v})$ is independent of x. If $Lv = \lambda v$, then $L\bar{v} = \bar{\lambda}\bar{v}$, so $W(u,v) = \text{const}$.

<u>Green functions, or fundamental solutions</u>.

We will use the method of "variation of constants" to solve the forced spectral problem $(L-\lambda)u = f$, or

$$(+) \qquad -u'' + (q(x) - \lambda)u = f(x)$$

Let $u_1(x)$ and $u_2(x)$ be independent solutions of the homogeneous equation $-u'' + (q(x) - \lambda)u = 0$, so $W(u_1, u_2) = \text{const} \neq 0$.

We seek a solution of (+) in the form

$$u(x) = c_1(x)\, u_1(x) + c_2(x)\, u_2(x).$$

By requiring

$$(++) \qquad c_1'(x)\, u_1(x) + c_2'(x)\, u_2(x) = 0,$$

we obtain

$$u''(x) = c_1(x)\, u_1''(x) + c_2(x)\, u_2''(x) + c_1'(x)\, u_1'(x) + c_2'(x)\, u_2'(x)$$

Now applying the ODE (†), we obtain

$$c_1'(x)\,u_1'(x) + c_2'(x)\,u_2'(x) = -f(x).$$

Thus, together with the assumption (††) yields the system

$$\begin{bmatrix} u_1(x) & u_2(x) \\ u_1'(x) & u_2'(x) \end{bmatrix} \begin{bmatrix} c_1'(x) \\ c_2'(x) \end{bmatrix} = \begin{bmatrix} 0 \\ -f(x) \end{bmatrix}$$

for $c_1'(x)$ and $c_2'(x)$; the solution is

$$\begin{cases} c_1'(x) = \dfrac{1}{W(u_1,u_2)}\, u_2(x) f(x) \\[2ex] c_2'(x) = \dfrac{-1}{W(u_1,u_2)}\, u_1(x) f(x) \end{cases}$$

$$\Longrightarrow \begin{cases} c_1(x) = c_1 + \dfrac{1}{W(u_1,u_2)} \displaystyle\int_{x_2}^{x} u_2(y) f(y)\,dy \\[2ex] c_2(x) = c_2 - \dfrac{1}{W(u_1,u_2)} \displaystyle\int_{x_1}^{x} u_1(y) f(y)\,dy \end{cases}$$

The solution of the forced spectral problem (†) is therefore

$$u(x) = c_1 u_1(x) + c_2 u_2(x) + \frac{1}{W(u_1,u_2)}\left[\int_{x_2}^{x} u_1(x) u_2(y) f(y)\,dy - \int_{x_1}^{x} u_2(x) u_1(y) f(y)\,dy\right] \qquad (**)$$

$$= c_1 u_1(x) + c_2 u_2(x) + u_p(x)$$

The particular solution $u_p(x)$ depends on the choice of solution basis $\{u_1, u_2\}$ and the choice of the fixed integration limits x_1 and x_2.

If we are interested in solving (†) in the interval $[x_1, x_2]$, the general solution (**) can be written as

$$u(x) = c_1 u_1(x) + c_2 u_2(x) + \int_{x_1}^{x_2} G(x,y)\, f(y)\, dy$$

with the kernel $G(x,y)$ given, for $x, y \in [x_1, x_2]$

$$G(x,y) = \frac{1}{W(u_1,u_2)} \tilde{G}(x,y) = \frac{1}{W(u_1,u_2)} \begin{cases} u_1(x) u_2(y), & x < y \\ u_2(x) u_1(y), & x > y \end{cases}$$

Notice that, for fixed $y \in (x_1, x_2)$,

$$\frac{d}{dx} G(x,y) = \frac{1}{W(u_1,u_2)} \begin{cases} u_1'(x) u_2(y), & x < y \\ u_2'(x) u_1(y), & x > y \end{cases},$$

and taking limits as $x \to y^-$ and $x \to y^+$,

$$\lim_{h \to 0^+} \left(\frac{d}{dx} G(y+h, y) - \frac{d}{dx} G(y-h, y) \right) = \frac{u_2'(y) u_1(y) - u_1'(y) u_2(y)}{W(u_1,u_2)}$$

$$= -1$$

If the ODE (+) is posed on the whole real line, then one may take x_1 and x_2 to be $-\infty$ and make an assumption on f, such as $f(x)=0$ for $x<x_0$ for some $x_0 \in \mathbb{R}$. Then the particular solution in (**) becomes

$$u_p(x) = \frac{1}{W(u_1,u_2)} \int_{-\infty}^{x} \left(u_1(x)u_2(y) - u_2(x)u_1(y)\right) f(y)\,dy$$

$$= \int_{-\infty}^{\infty} \Phi_c(x,y)\, f(y)\,dy,$$

in which the kernel $\Phi_c(x,y)$ is

$$\Phi_c(x,y) = \frac{1}{W(u_1,u_2)} \begin{cases} u_1(x)u_2(y) - u_2(x)u_1(y), & x>y \\ 0, & x<y \end{cases}$$

and the subscript "c" stands for "causal".

Notice that

$$\lim_{h\to 0^+}\left(\frac{d}{dx}\Phi_c(y+h,y) - \frac{d}{dx}\Phi_c(y-h,y)\right) = -1$$

When the potential vanishes, i.e., $q(x)=0$, we can take $u_1(x) = e^{-i\sqrt{\lambda}x}$ and $u_2(x) = e^{+i\sqrt{\lambda}x}$, so that $W(u_1,u_2) = +2i\sqrt{\lambda}$, and we obtain, for $\lambda \neq 0$,

$$\Phi_c(x,y) = \begin{cases} -\frac{1}{\sqrt{\lambda}} \sin\sqrt{\lambda}(x-y), & x>y \\ 0, & x<y \end{cases}$$

The <u>resolvent Green function</u> :

Again with $\underset{\sim}{q(x) = 0}$ and $u_1(x;\lambda) = e^{-i\sqrt{\lambda}x}$ and $u_2(x;\lambda) e^{i\sqrt{\lambda}x}$, and $\operatorname{Im}\sqrt{\lambda} > 0$ for $\lambda \neq 0$, let us take $x_1 = -\infty$ and $x_2 = \infty$. Then the formula in (**) becomes

$$u_p(x) = \int_{-\infty}^{\infty} \overset{\circ}{R}(x, y; \lambda) f(y)\, dy ,$$

where $\overset{\circ}{R}(x, y; \lambda) = \dfrac{-1}{2i\sqrt{\lambda}} e^{i\sqrt{\lambda}|x-y|}$.

By the choice of $\sqrt{\lambda}$, $R(x, y, \lambda)$ is exponentially decaying as a function of the separation $|x-y|$ between "source" and "influence" points y and x.

For a <u>confined (real) potential</u> $q(x)$, with $q(x) = 0$ for $|x| > L \in \mathbb{R}$ and $q \in L^2(\mathbb{R})$, there are solutions u_1 and u_2 with the properties

$$u_1(x;\lambda) = e^{-i\sqrt{\lambda}x} \quad \text{for } x < -L$$
$$u_2(x;\lambda) = e^{i\sqrt{\lambda}x} \quad \text{for } x > L$$

I will leave it as an <u>exercise</u> to prove that such solutions do exist — use the Volterra theory.

Define $W(\lambda) := \det \begin{bmatrix} u_1(x;\lambda) & u_2(x;\lambda) \\ u_1'(x;\lambda) & u_2'(x;\lambda) \end{bmatrix}$,

with primes denoting x-derivatives.

The particular soln in (**), with $x_1 = -\infty$ and $x_2 = \infty$, is

$$u_p(x) = \int_{-\infty}^{\infty} R(x,y;\lambda) f(y)\, dy ,$$

in which the resolvent kernel $R(x,y;\lambda)$ is

$$R(x,y;\lambda) = \frac{-1}{W(\lambda)} \begin{cases} u_+(y;\lambda)\, u_-(x;\lambda), & x \le y \\ u_-(y;\lambda)\, u_+(x;\lambda), & x \ge y \end{cases} = \frac{-1}{W(\lambda)} \tilde{R}(x,y;\lambda)$$

The function $W(\lambda)$ is analytic in the slit complex plane $\mathbb{C} \setminus [0,\infty)$. This will be proved through a sequence of exercises in the next assignment.

In fact, $W(\lambda) \neq 0$ for all $\lambda \in \mathbb{C} \setminus \mathbb{R}$. This is quite easy to prove: If $W(\lambda) = 0$, then $u_2(x;\lambda) = \beta\, u_1(x,\lambda)$ for some $\beta \neq 0$. Thus

$$\begin{aligned} u_2(x;\lambda) &= \beta e^{-i\sqrt{\lambda}\, x} && \text{for } x < -L \\ u_2(x;\lambda) &= e^{i\sqrt{\lambda}\, x} && \text{for } x > L . \end{aligned}$$

With $L = -\frac{d^2}{dx^2} + q(x)$ and q real-valued,

$$\lambda \int |u_2|^2 = \int (Lu_2)\overline{u_2} = \int u_2 (\overline{Lu_2}) = \bar{\lambda} \int |u_2|^2 < \infty$$

$$\Longrightarrow \quad \lambda = \bar{\lambda} \quad \Longrightarrow \quad \lambda \in \mathbb{R} .$$

Now consider the Schrödinger operator on the line with a potential of bounded support:

$$L = -\frac{d^2}{dx^2} + q(x),$$

where $q(x) = 0$ for $|x| \geq L$ $(L > 0)$.
Assume that q is real-valued and square-integrable.

For $\lambda \in \mathbb{C} \setminus [0,\infty)$, let solutions $u_\pm(x;\lambda)$ of $-u'' + (q(x) - \lambda)u = 0$ be defined by

$$u_-(x;\lambda) = e^{-i\sqrt{\lambda}\,x} \qquad \text{for} \quad x < -L$$
$$u_+(x;\lambda) = e^{i\sqrt{\lambda}\,x} \qquad \text{for} \quad x > L$$

The Wronskian of these is independent of x,

$$W(\lambda) := \det \begin{bmatrix} u_-(x,\lambda) & u_+(x,\lambda) \\ u_-'(x,\lambda) & u_+'(x,\lambda) \end{bmatrix},$$

and it is analytic in λ in $\mathbb{C} \setminus [0,\infty)$. The resolvent Green function is

$$R(x,y;\lambda) = -\frac{1}{W(\lambda)} \begin{cases} u_+(x;\lambda)\, u_-(x;\lambda), & x \leq y \\ u_-(x;\lambda)\, u_+(x;\lambda), & x \geq y \end{cases}$$

$$= -\frac{1}{W(\lambda)} \tilde{R}(x,y;\lambda).$$

Eigenvalues of L.

We define an eigenvalue of L to be a number $\lambda \in \mathbb{C}$ such that there exists a function $u \in L^2(\mathbb{R})$ such that $-u'' + (q(x) - \lambda)u = 0$. This function, as we have seen from the Volterra theory, is necessarily absolutely continuous, and it is the eigenfunction for the eigenvalue λ.

An eigenvalue of λ is necessarily a negative real number: To wit: Let $-u'' + (q(x) - \lambda)u = 0$ for some $u \in L^2(\mathbb{R})$. Then $\lambda(u,u) = (\lambda u, u) = (Lu, u) = (u, Lu) = (u, \lambda u) = \bar{\lambda}(u,u)$ $\Rightarrow \lambda = \bar{\lambda} \Rightarrow \lambda \in \mathbb{R}$. To see that $\lambda < 0$, observe that, for $x > L$, $u(x) = ae^{i\sqrt{\lambda}x} + be^{-i\sqrt{\lambda}x}$ with a and b not both zero and $i\sqrt{\lambda}$ is purely imaginary. It follows that u is not square integrable.

The solutions u_- and u_+ have the following behavior for $|x| > L$:

(*)

$$u_-(x;\lambda) = \begin{cases} e^{-i\sqrt{\lambda}x}, & x \le -L \\ a(\lambda)e^{i\sqrt{\lambda}x} + b(\lambda)e^{-i\sqrt{\lambda}x}, & x \ge L \end{cases}$$

$$u_+(x;\lambda) = \begin{cases} c(\lambda)e^{-i\sqrt{\lambda}x} + d(\lambda)e^{i\sqrt{\lambda}x}, & x \le -L \\ e^{i\sqrt{\lambda}x}, & x \ge L \end{cases}$$

Both $u_-(x;\lambda)$ and $u_+(x;\lambda)$ are real-valued for $\lambda < 0$.
Prove this.

The following proposition is easy enough to prove (do it):

<u>Proposition</u> λ_0 is an eigenvalue of $-\frac{d^2}{dx^2} + q(x)$ if and only if $b(\lambda_0) = 0$ and if and only if $d(\lambda) = 0$ and if and only if $W(\lambda_0) = 0$. The associated eigenfunction is exponentially decaying as $|x| \to \infty$.

If λ_0 is an eigenvalue of L, then

$$u_+(x;\lambda_0) = \beta u_-(x;\lambda_0), \tag{**}$$

and $c(\lambda_0) = \beta$, $d(\lambda_0) = 0$, $a(\lambda_0) = \beta^{-1}$, and $b(\lambda_0) = 0$. Define α to be the square L^2-norm of u_-:

$$\alpha = \int_{\mathbb{R}} u_-(x;\lambda_0)^2 \, dx.$$

<u>Theorem</u> The set of roots of $W(\lambda)$ is a finite subset of $(-\infty, 0)$. Let λ_0 be a root of $W(\lambda)$.

1. $\lambda_0 \geq \min_{x\in\mathbb{R}} q(x)$
2. $W'(\lambda_0) = -\beta\alpha$
3. The residue of the kernel $R(x,y;\lambda)$ at λ_0 is

$$\operatorname{Res}\Big|_{\lambda_0} R(x,y;\lambda) = \frac{\tilde{R}(x,y;\lambda_0)}{\beta\alpha} = \frac{u_-(x)\,u_-(y)}{\alpha^2}$$

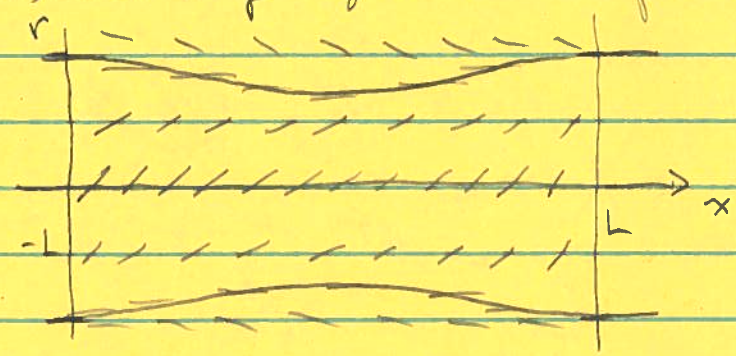
Proof

I will not prove the finiteness of the set of roots of W here.

1. Let u satisfy $-u'' + (q(x) - \lambda)u = 0$, and set $r(x) = u'(x)/u(x)$. Then r satisfies the ODE

$$r'(x) = -r(x)^2 + (q(x) - \lambda)$$

as long as $u(x) \neq 0$. ($u(x) = 0$ occurs at a vertical asymptote of the graph of $r(x)$.) The following phase-plane argument can be made precise: The slope field for the ODE for r, assuming $q(x) - \lambda > 0$ for all $x \in \mathbb{R}$, looks like



The two solid lines are the zero set of the right-hand side of the ODE for r, i.e., where

$$r^2 = q(x) - \lambda .$$

It is clear from the picture (and can be made precise by an easy but maybe technical argument) that, if $r(-L) > 0$, then $r(L) > 0$ also.

But, if u is an eigenfunction of L, then by $(*)$ and $(**)$, $r(-L) = -i\sqrt{\lambda_0} > 0$ and $r(L) = i\sqrt{\lambda_0} < 0$.

Thus $q(x) - \lambda_0$ cannot be uniformly positive on $\mathbb{R}$, and the statement 1 follows.

2. Let λ_0 be an eigenvalue of L, ie $W(\lambda_0) = 0$.

From the ODE $-u_\pm'' + q(x) u_\pm = \lambda u_\pm$, one obtains

$$\frac{d}{dx} \det \begin{bmatrix} u_-(x;\lambda_0) & u_+(x;\lambda) \\ u_-'(x;\lambda_0) & u_+'(x;\lambda) \end{bmatrix} = (\lambda_0 - \lambda)\, u_-(x;\lambda_0) u_+(x;\lambda)$$

Integrating over an interval $[-x, x)$ with $x > L$ yields

$$i(a(\lambda) + \beta)(\sqrt{\lambda_0} - \sqrt{\lambda})\, e^{i(\sqrt{\lambda_0} - \sqrt{\lambda})x} + i b(\lambda)(\sqrt{\lambda_0} + \sqrt{\lambda})\, e^{i(\sqrt{\lambda_0} - \sqrt{\lambda})x}$$

$$= (\lambda_0 - \lambda) \int_{-x}^{x} u_-(y;\lambda_0) u_+(y;\lambda)\, dy .$$

Dividing by $(\lambda_0 - \lambda)$ yields

$$\frac{i(a(\lambda) + \beta)}{\sqrt{\lambda_0} + \sqrt{\lambda}} e^{i(\sqrt{\lambda_0} - \sqrt{\lambda})x} + \frac{i b(\lambda)}{\sqrt{\lambda_0} - \sqrt{\lambda}} e^{i(\sqrt{\lambda_0} - \sqrt{\lambda})x} = \int_{-x}^{x} u_- u_+ \, dy$$

Taking the limit as $\lambda \to \lambda_0$ yields (recall $b(\lambda_0) = 0$)

$$\frac{i(\beta^{-1} + \beta)}{2\sqrt{\lambda_0}} e^{2i\sqrt{\lambda_0}\, x} - 2i\sqrt{\lambda_0}\, b'(\lambda_0) = \beta \int_{-x}^{x} u_-(y;\lambda_0)^2 \, dy$$

Now, taking $x \to \infty$ yields

$$-2i\sqrt{\lambda_0}\, b'(\lambda_0) = \beta\alpha .$$

By computing $W(\lambda)$ using $x > L$ and the form $(*)$, we obtain

$$W(\lambda) = 2i\sqrt{\lambda}\, b(\lambda)$$

Using $W(\lambda_0) = 0$ yields

$$W'(\lambda_0) = 2i\sqrt{\lambda_0}\, b'(\lambda_0)$$

and therefore $W'(\lambda_0) = -\beta\alpha$.

3. Now the residue of $R(x,y;\lambda)$ at λ_0 can be computed:

$$\mathrm{Res}\big|_{\lambda=\lambda_0} R(x,y;\lambda) = -\frac{\tilde{R}(x,y;\lambda_0)}{W'(\lambda_0)} = \frac{\tilde{R}(x,y;\lambda_0)}{\alpha\beta}$$

That this is equal to $u_-(x;\lambda_0)u_-(y;\lambda_0)/\alpha^2$ is easy to show. $\boxtimes$