AMATH 568
Advanced Differential Equations
Homework 2

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1. *Particle in a box:* Consider the time-independent Schrödinger equation:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi$$

which is the underlying equation of quantum mechanics where $V(x)$ is a given potential.

(a) Let $\psi = u(x)\exp(-iEt/\hbar)$ and derive the time-independent Schrödinger equation. (Note that E here corresponds to energy).

Solution: Substituting $\psi = ue^{-iEt/\hbar}$ we find the following

$$i\hbar\frac{\partial}{\partial t}\left(ue^{-iEt/\hbar}\right) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\left(ue^{-iEt/\hbar}\right) + V(x)ue^{-iEt/\hbar}$$

$$\Rightarrow Eue^{-iEt/\hbar} = \left[-\frac{\hbar^2}{2m}u_{xx} + V(x)u\right]e^{-iEt/\hbar}$$

$$\Rightarrow Eu = -\frac{\hbar^2}{2m}u_{xx} + V(x)u$$

which is the time-independent Schrödinger equation.

(b) Show that the resulting eigenvalue problem is of Sturm-Liouville type.

Solution: Recall that a Sturm-Liouville type problem is one which can be written in the form

$$Lu = \mu r(x)u + f(x)$$

with Robin boundary conditions on the domain $x \in [a, b]$ and with the operator L taking the form

$$Lu = -\frac{\partial}{\partial x}\left[p(x)\frac{\partial u}{\partial x}\right] + q(x)u$$

Comparing this expression with the TISE derived above, we see that it is a Sturm-Liouville problem with the following parameters:

$$p(x) = \frac{\hbar^2}{2m} \qquad q(x) = V(x) \qquad r(x) = 1 \qquad \mu = E \qquad f(x) = 0$$

(c) Consider the potential

$$V(x) = \begin{matrix} 0 & |x| < L \\ \infty & \text{elsewhere} \end{matrix}$$

which implies $u(L) = u(-L) = 0$. Calculate the normalized eigenfunctions and eigenvalues.

Solution: For $x \in [-L, L]$ we have $V(x) = 0$ and so our equation takes the form

$$-\frac{\hbar^2}{2m}u_{xx} = Eu \Rightarrow u_{xx} = \frac{-2mE}{\hbar^2}u$$

This is an ODE whose general solution is given by

$$u(x) = A\sin\left(\frac{\sqrt{2mE}}{\hbar}x\right) + B\cos\left(\frac{\sqrt{2mE}}{\hbar}x\right) = A_1\sin\left(\frac{\sqrt{2mE}}{\hbar}(x - A_2)\right)$$

Our chosen potential imposes the boundary conditions $u(-L) = u(L) = 0$. We can satisfy the left-hand boundary condition by setting $A_2 = -L$, while the second condition is satisfied when

$$\frac{\sqrt{2mE}}{\hbar}(2L) = n\pi \Rightarrow E = \frac{n^2\hbar^2\pi^2}{8mL^2}$$

Where n is an integer. Hence, we find our energy can only take on discrete values E_n, and our general solution is given by

$$u_n(x) = A\sin\left(\frac{n\pi}{2L}(x + L)\right) \qquad n \in \{1, 2, \dots\}$$

Lastly, we normalize this function by requiring that $\langle u_n, u_n\rangle = 1$. This gives us

$$\langle u_n, u_n\rangle = |A|^2\int_{-L}^{L}\sin^2\left(\frac{n\pi}{2L}(x + L)\right)dx = |A|^2 L$$

Hence, for $\langle u_n, u_n \rangle = 1$ we require that $|A|^2 L = 1 \Rightarrow A = \frac{1}{\sqrt{L}}$. Putting it all together, we find the normalized eigenfunctions and eigenvalues to be

$$u_n(x) = \frac{1}{\sqrt{L}} \sin\left(\frac{n\pi}{2L}(x+L)\right) \qquad E_n = \frac{n^2\hbar^2\pi^2}{8mL^2} \qquad n \in \{1, 2, \dots\}$$

(d) If an electron jumps from the third state to the ground state, what is the frequency of the emitted photon? Recall that $E = \hbar\omega$.

Solution: We have the following energies for the third and ground state:

$$E_1 = \frac{\hbar^2\pi^2}{8mL^2} \qquad E_3 = \frac{9\hbar^2\pi^2}{8mL^2}$$

By conservation of energy, the emitted photon will carry energy equal to the difference between these two levels. Hence we have

$$\hbar\omega = E_3 - E_1 = \frac{\hbar^2\pi^2}{mL^2} \qquad \Rightarrow \qquad \omega = \frac{\hbar\pi^2}{mL^2}$$

(e) If the box is cut in half, then $u(0) = u(L) = 0$. What are the resulting eigenfunctions and eigenvalues?

Solution: Looking at our solution set for the original problem, we note that when n is even we have $u_n(0) = u_n(L) = 0$, so these solutions satisfy our updated boundary conditions. Hence if we replace n with $2n$ we have a set of functions which satisfy our conditions.

All that remains now is to re-normalize our solutions. We note that $|u_n(x)|^2$ is symmetric about the origin, so $\int_0^L |u_n(x)|^2 dx = \frac{1}{2}\int_{-L}^{L} |u_n(x)|^2 dx = \frac{1}{2}$. Therefore, to re-normalize our functions we need the square of our normalization constant to be twice as large. This leads us to the new set of eigenfunctions and eigenvalues:

$$u_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}(x+L)\right) \qquad E_n = \frac{n^2\hbar^2\pi^2}{2mL^2} \qquad n \in \{1, 2, \dots\}$$

2. Find the Green's function (fundamental solution) for each of the following problems, and express the solution u in terms of the Green's function.

(a) $u'' + c^2 u = f(x)$ with $u(0) = u(L) = 0$.

Solution: This is a Sturm-Liouville function with $p(x) = -1$ and $q(x) = c^2$. The Green's function for this problem satisfies

$$G_{xx} + c^2 G = \delta(x-\xi) \qquad\qquad G(0) = G(L) = 0$$

For $x \neq \xi$, this reduces to the homogeneous ODE

$$G_{xx} = -c^2 G$$

which has the general solution

$$G(x) = A\sin(cx + B)$$

For $x < \xi$ the solution which satisfies the boundary condition $G(0) = 0$ is $G(x) = A\sin cx$. For $x > \xi$, the solution which satisfies the boundary condition $G(L) = 0$ is $G(x) = B\sin(c(x-L))$.
We require that the left and right solutions satisfy the additional constraints $[G]_\xi = 0$ and $[G_x]_\xi = -\frac{1}{p(x)} = 1$.

$$\begin{aligned} [G]_\xi = 0 \qquad &\Rightarrow \qquad & A\sin(c\xi) = B\sin(c(\xi - L)) \\ [G_x]_\xi = 1 \qquad &\Rightarrow \qquad & Bc\cos(c(\xi-L)) - Ac\cos(c\xi) = 1 \end{aligned}$$

We can use the trigonometric identities $\sin(a+b) = \sin a\cos b + \sin b\cos a$ and $\cos(a+b) = \cos a\cos b - \sin a\sin b$ to rewrite these expressions. The first equation gives us

$$A\sin(c\xi) = B[-\sin(c\xi)\cos(cL) + \sin(cL)\cos(c\xi)]$$

$$\Rightarrow A + B\cos(cL) = B\frac{\sin(cL)}{\tan(c\xi)}$$

while the second equation results in

$$Bc[-\cos(c\xi)\cos(cL) - \sin(c\xi)\sin(cL)] - Ac\cos(c\xi) = 1$$

$$\Rightarrow 1 + c\cos(c\xi)[A + B\cos(cL)] = -Bc\sin(c\xi)\sin(cL)$$

Plugging in the expression found for $A + B\cos(cL)$ into the second equation results in

$$\begin{aligned} 1 + c\cos(c\xi)\frac{B\sin(cL)}{\tan(c\xi)} &= -Bc\sin(c\xi)\sin(cL) \\ \Rightarrow \sin(c\xi) + Bc\sin(cL) &= 0 \\ \Rightarrow B = \frac{-\sin(c\xi)}{c\sin(cL)} &\qquad A = \frac{-\sin(c(\xi-L))}{c\sin(cL)} \end{aligned}$$

And so we find the Green's function to be

$$G(x,\xi) = \begin{cases} -\sin(cx)\sin(c(\xi-L))/(c\sin(cL)) & x<\xi \\ \\ -\sin(c(x-L))\sin(c\xi)/(c\sin(cL)) & x>\xi \end{cases}$$

The final solution can be found by performing the following integration

$$u(x) = \int_0^L f(\xi)G(\xi,x)d\xi$$

(b) $u'' - c^2u = f(x)$ with $u(0) = u(L) = 0$.
Solution: This is a Sturm-Liouville problem with $p(x) = -1$ and $q(x) = -c^2$. The Green's function for this problem satisfies

$$G'' - c^2G = \delta(x-\xi) \qquad\qquad G(0) = G(L) = 0$$

For $x \neq \xi$, we have $G'' = c^2G$, which has solutions of the form

$$y(x) = Ae^{cx} + Be^{-cx}$$

Hence we have

i. $x < \xi$: The solution which satisfies the left boundary condition $G(0) = 0$ is given by
$$G = Ae^{cx} - Ae^{-cx} = A\sinh(cx)$$

ii. $x > \xi$: The solution satisfying the right boundary condition $G(L) = 0$ is given by
$$G = Be^{c(x-L)} - Be^{-c(x-L)} = B\sinh(c(x-L))$$

Next, we require that the Green's function satisfy the additional constraints $[G]_\xi = 0$ and $[G_x]_\xi = -\frac{1}{p(x)} = 1$.

$$\begin{aligned} [G]_\xi = 0 \qquad &\Rightarrow \qquad A\sinh(c\xi) = B\sinh(c(\xi-L)) \\ [G_x]_\xi = 1 \qquad &\Rightarrow \qquad Bc\cosh(c(\xi-L)) - Ac\cosh(c\xi) = 1 \end{aligned}$$

This system of equation is almost identical to the ones for part (a) but with hyperbolic trig functions. We will use the trigonometric identities $\sinh(a+b) = \sinh a\cosh b + \sinh b\cosh a$ and $\cosh(a+b) = \cosh a\cosh b - \sinh a\sinh b$ to rewrite these expressions. The first equation gives us

$$A\sinh(c\xi) = B[-\sinh(c\xi)\cosh(cL) + \sinh(cL)\cosh(c\xi)]$$

$$\Rightarrow A + B\cosh(cL) = B\frac{\sinh(cL)}{\tanh(c\xi)}$$

while the second equation results in

$$Bc[-\cosh(c\xi)\cosh(cL) - \sinh(c\xi)\sinh(cL)] - Ac\cosh(c\xi) = 1$$

$$\Rightarrow 1 + c\cosh(c\xi)[A + B\cosh(cL)] + Bc\sinh(c\xi)\sinh(cL) = 0$$

Plugging in the expression found for $A + B\cos(cL)$ into the second equation results in

$$1 + Bc\cosh(c\xi)\frac{\sinh(cL)}{\tanh(c\xi)} + Bc\sinh(c\xi)\sinh(cL) = 0$$

$$\Rightarrow \sinh(c\xi) + Bc\sinh(cL)[\cosh^2(c\xi) + \sinh^2(c\xi)] = 0$$

We now use $\sinh^2 x + \cosh^2 x = \cosh(2x)$ to simplify this expression, resulting in the following expressions for our A and B coefficients.

$$\Rightarrow B = -\frac{\sinh(c\xi)}{c\sinh(cL)\cosh(2c\xi)} \qquad A = -\frac{\sinh(c(\xi - L))}{c\sinh(cL)\cosh(2c\xi)}$$

Hence, our Green's function solution is given by

$$G(x,\xi) = \begin{cases} -\sinh(c(\xi - L))\sinh(cx)/(c\sinh(cL)\cosh(2c\xi)) & x < \xi \\ -\sinh(c\xi)\sinh(c(x - L))/(c\sinh(cL)\cosh(2c\xi)) & x > \xi \end{cases}$$

The final solution can be found by performing the following integration

$$u(x) = \int_0^L f(\xi)G(\xi,x)d\xi$$

3. Calculate the solution of the Sturm-Liouville problem using the Green's function approach.

$$Lu = -[p(x)u_x]_x + q(x)u = f(x) \qquad 0 \leq x \leq L$$

with

$$\alpha_1 u(0) + \beta_1 u'(0) = 0 \qquad \text{and} \qquad \alpha_2 u(L) + \beta_2 u'(L) = 0$$

Solution: To solve a general Sturm-Liouville problem using the Green's function approach, we seek a function satisfying

$$LG = -[p(x)G_x]_x + q(x)G = \delta(x-\xi)$$

on the interval $x, \xi \in [0, L]$, satisfying the boundary conditions

$$\alpha_1 G(0) + \beta_1 G_x(0) = 0 \qquad \text{and} \qquad \alpha_2 G(L) + \beta_2 G_x(L) = 0$$

We also require that G is continuous within its domain. This results in the additional constraint

$$[G(x,\xi)]_\xi = G(\xi^+, \xi) - G(\xi^-, \xi) = 0$$

Lastly, we impose a jump in the derivative of G at the ξ, which can be found by integrating our equation over the small interval containing ξ. This gives us

$$\begin{aligned}\int_{\xi^-}^{\xi^+} (-[p(x)G_x]_x + q(x)G)dx &= \int_{\xi^-}^{\xi^+} \delta(x-\xi)dx \\ -[p(x)G_x]_{\xi^-}^{\xi^+} + \int_{\xi^-}^{\xi^+} q(x)Gdx &= 1\end{aligned}$$

$$[p(x)G_x]_\xi = -1 \Rightarrow [G_x(x,\xi)]_\xi = -\frac{1}{p(\xi)}$$

With these conditions in mind, we can proceed by solving the associated homogeneous problem for the two regimes $x < \xi$ and $x > \xi$. For $x < \xi$ we will solve $LG = 0$ with the left boundary condition enforced, to produce a solution

$$G = Ay_1(x) \qquad\qquad x < \xi$$

Similarly, for $x > \xi$ we will solve $LG = 0$ with the right boundary condition enforced to produce a solution

$$G = By_2(x) \qquad\qquad x > \xi$$

We are left with two remaining degrees of freedom in the coefficients A and B, and we can use our two additional constraints to solve for these.

Our continuity condition requires that

$$[G]_\xi = By_2(\xi) - Ay_1(\xi) = 0 \Rightarrow B = A\frac{y_1(\xi)}{y_2(\xi)}$$

While our condition on the first derivative G_x requires that

$$[G_x]_\xi = By_2'(\xi) - Ay_1'(\xi) = -\frac{1}{p(\xi)}$$

Applying the first equation to the second results in

$$A\frac{y_1(\xi)}{y_2(\xi)}y_2'(\xi) - Ay_1'(\xi) = -\frac{1}{p(\xi)} \Rightarrow A = -\frac{y_2(\xi)}{p(\xi)W(\xi)}$$

Where $W(\xi)$ is the Wronskian between $y_1(x)$ and $y_2(x)$ evaluated at $x = \xi$. Plugging in these expressions for our coefficients, we can write down the final Green's function as

$$G(x,\xi) = \begin{cases} -y_1(x)y_2(\xi)/(p(\xi)W(\xi)) & x < \xi \\ \\ -y_1(\xi)y_2(x)/(p(\xi)W(\xi)) & x > \xi \end{cases}$$

With this Green's function, we may calculate the solution to any Sturm-Liouville problem by computing the integral

$$u(x) = \int_0^L f(\xi)G(\xi,x)d\xi$$