Homework 3
Due: February 3, 2021

1. *Particle in a box*: Consider the time-dependent 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).
(b) Show that the resulting eigenvalue problem is of Sturm-Liouville type.
(c) Consider the potential

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

which implies $u(L) = u(-L) = 0$. Calculate the normalized eigenfunctions and eigenvalues.
(d) What is the energy of the ground state (the lowest energy state $\neq 0$)
(e) If an electron jumps from the third state to the ground state, what is the frequency of the emitted photon. Recall that $E = \hbar\omega$.
(f) If the box is cut in half, then $u(0) = u(L) = 0$. What are the resulting eigenfunctions and eigenvalues (Think!)

Solution.
(a)

$$\begin{aligned}\frac{\partial\psi}{\partial t} &= \frac{-iE}{\hbar}u(x)\exp(-iEt/\hbar)\\ \frac{\partial^2\psi}{\partial x^2} &= u''(x)\exp(-iEt/\hbar)\end{aligned}$$

Substituting to the equation

$$\begin{aligned}i\hbar\frac{-iE}{\hbar}u(x)\exp(-iEt/\hbar) &= -\frac{\hbar^2}{2m}u''(x)\exp(-iEt/\hbar) + V(x)u(x)\exp(-iEt/\hbar)\\ Eu(x) &= -\frac{\hbar^2}{2m}u''(x) + V(x)u(x)\end{aligned}$$

(b) Consider the general Sturm-Liouville problem and our problem

$$\begin{aligned}-\frac{d}{dx}\left(p(x)\frac{du}{dx}\right) + q(x)u &= \mu r(x)u + f(x)\\ -\frac{d}{dx}\left(\frac{du}{dx}\right) + \frac{2m}{\hbar^2}V(x)u &= \frac{2mE}{\hbar^2}u\end{aligned}$$

Then $p(x) = 1, q(x) = \frac{2m}{\hbar^2}V(x), \mu = \frac{2mE}{\hbar^2}, r(x) = 1, f(x) = 0.$

(c) The eigenvalue problem assocaited with this problem is

$$u'' + \lambda_n u = 0, \quad \lambda_n = \frac{2mE}{\hbar^2}$$

which has a general solution

$$u = c_1 \sin(\sqrt{\lambda_n}x) + c_2 \cos(\sqrt{\lambda_n}x)$$

Consider BCs, $u(L) = u(-L) = 0$

$$\begin{aligned} c_1 \sin(\sqrt{\lambda_n}L) + c_2 \cos(\sqrt{\lambda_n}L) = 0 \\ -c_1 \sin(\sqrt{\lambda_n}L) + c_2 \cos(\sqrt{\lambda_n}L) = 0 \end{aligned}$$

Adding these equations we get $2c_2 \cos(\sqrt{\lambda_n}L) = 0 \to \sqrt{\lambda_n}L = (n + 1/2)\pi$. Thus $\sqrt{\lambda_n} = \frac{(n+1/2)\pi}{L}$ for $n = 0, 1, \cdots$. The BCs also imply that $\sin(\sqrt{\lambda_n}L) = 0$, then $\sqrt{\lambda_n}L = n\pi$ and $\sqrt{\lambda_n} = \frac{n\pi}{L}$ for $n = 1, 2, \cdots$. Now consider the inner product

$$\begin{aligned} \langle c_1 \sin(\sqrt{\lambda_n}x), c_1 \sin(\sqrt{\lambda_n}x)\rangle &= c_1^2 \int_{-L}^{L} \sin^2(\frac{n\pi x}{L})dx \\ &= \frac{c_1^2}{2}\int_{-L}^{L} 1 - \cos\left(\frac{2n\pi x}{L}\right) dx \\ &= \frac{c_1^2}{2}\left[x - \frac{L}{2n\pi}\sin\left(\frac{2n\pi x}{L}\right)\right]_{-L}^{L} \\ &= \frac{c_1^2}{2}\cdot 2L \\ &= c_1^2 L = 1 \to c_1 = \sqrt{\frac{1}{L}} \end{aligned}$$

Similarly for the cosine function

$$\begin{aligned} \langle c_2 \cos(\sqrt{\lambda_n}x), c_2 \cos(\sqrt{\lambda_n}x)\rangle &= c_2^2 \int_{-L}^{L} \cos^2(\frac{(n+1/2)\pi x}{L})dx \\ &= \frac{c_2^2}{2}\int_{-L}^{L} 1 - \cos\left(\frac{(2n+1)\pi x}{L}\right) dx \\ &= \frac{c_2^2}{2}\left[x - \frac{L}{(2n+1)\pi}\sin\left(\frac{(2n+1)\pi x}{L}\right)\right]_{-L}^{L} \\ &= \frac{c_2^2}{2}\cdot 2L \\ &= c_2^2 L = 1 \to c_2 = \sqrt{\frac{1}{L}} \end{aligned}$$

Thus the normalized eigenfunction is

$$u(x) = \sqrt{\frac{1}{L}} \sum_{n=1}^{\infty} \sin\left(\frac{n\pi x}{L}\right) + \sqrt{\frac{1}{L}} \sum_{n=0}^{\infty} \cos\left(\frac{(n+1/2)\pi x}{L}\right)$$

(d) The ground state is at $n = 0$. Since $\lambda_n = \frac{2mE}{\hbar^2}$

$$\left(\frac{1/2\pi}{L}\right)^2 = \frac{2mE_0}{\hbar^2}$$
$$E_0 = \frac{\pi^2\hbar^2}{8mL}$$

(e) The third state is at $n = 1$ of the cosine function

$$\left(\frac{(1+1/2)\pi}{L}\right)^2 = \frac{2mE_2}{\hbar^2}$$
$$E_2 = \frac{9\pi^2\hbar^2}{8mL}$$

Thus the energy released is

$$\Delta E = E_2 - E_0 = \frac{\pi^2\hbar^2}{mL} = \hbar\omega \to \omega = \frac{\pi^2\hbar}{mL}$$

(f) If $u(0) = u(L) = 0$, we need to remove the cosine function since it does not satisfy BCs. Since the box is cut in half, the normalization constant is now $\frac{c^2}{2}L = 1 \to c = \sqrt{\frac{2}{L}}$. Thus the resulting eigenfunction is

$$u(x) = \sqrt{\frac{2}{L}} \sum_{n=1}^{\infty} \sin\left(\frac{n\pi x}{L}\right)$$

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 $u(0) = u(L) = 0$
(b) $u'' - c^2 u = f(x)$ with $u(0) = u(L) = 0$

Solution.
(a) The Green's function satisfies

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

In Sturm-Liouville form

$$-(p(x)G_x)_x + c^2 G = \delta(x - \xi), \quad p(x) = -1$$

Consider solution for $x < \xi$

$$G(0) = 0 \longrightarrow G = A\sin(cx) = Ay_1$$

For $x > \xi$

$$G(L) = 0 \longrightarrow G = B\sin(c(x - L)) = By_2$$

The Green's function also has to satisfy: (1) $[G]_\xi = 0$ (2) $[G_x]_\xi = -1/p(\xi)$. Imposing these restrictions gives (104) of Kutz notes

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

where the Wronskian is given by

$$W = y_1 y_2' - y_1' y_2 = c\sin(cx)\cos(c(x - L)) - c\cos(cx)\sin(c(x - L))$$

Substituting to the Green's function

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

Then u can be expressed as (note ξ and x can be used interchangeably)

$$\begin{aligned} u &= \int_0^L f(\xi)G(\xi, x)d\xi \\ &= \int_0^x \frac{-f(\xi)\sin(c\xi)\sin(c(x - L))d\xi}{c\sin(c\xi)\cos(c(\xi - L)) - c\cos(c\xi)\sin(c(\xi - L))} \\ &+ \int_x^L \frac{-f(\xi)\sin(cx)\sin(c(\xi - L))d\xi}{c\sin(c\xi)\cos(c(\xi - L)) - c\cos(c\xi)\sin(c(\xi - L))} \end{aligned}$$

(b) We follow the same procedure in (a). The Green's function satisfies

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

In Sturm-Liouville form

$$-(p(x)G_x)_x - c^2 G = \delta(x-\xi), \quad p(x) = -1$$

Consider solution for $x < \xi$

$$G(0) = 0 \longrightarrow G = A\sinh(cx) = Ay_1$$

For $x > \xi$

$$G(L) = 0 \longrightarrow G = B\sinh(c(x-L)) = By_2$$

The Green's function also has to satisfy: (1) $[G]_\xi = 0$ (2) $[G_x]_\xi = -1/p(\xi)$. Imposing these restrictions gives

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

where the Wronskian is given by

$$W = y_1 y_2' - y_1' y_2 = c\sinh(cx)\cosh(c(x-L)) - c\cosh(cx)\sinh(c(x-L))$$

Substituting to the Green's function

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

Then u can be expressed as

$$\begin{aligned} u &= \int_0^L f(\xi)G(\xi,x)d\xi \\ &= \int_0^x \frac{-f(\xi)\sinh(c\xi)\sinh(c(x-L))d\xi}{c\sinh(c\xi)\cosh(c(\xi-L)) - c\cosh(c\xi)\sinh(c(\xi-L))} \\ &+ \int_x^L \frac{-f(\xi)\sinh(cx)\sinh(c(\xi-L))d\xi}{c\sinh(c\xi)\cosh(c(\xi-L)) - c\cosh(c\xi)\sinh(c(\xi-L))} \end{aligned}$$

3. Calculate the solution of the Sturm-Liouville problem using the Green's function approach (See the notes as I already showed you what the answer should be)

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

with

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

Solution.

The Green's function satisfies

$$LG = -\left[p(x)G_x\right]_x + q(x)G = \delta(x-\xi) \tag{1}$$

with boundary conditions

$$\begin{aligned} \alpha_1 G(0) + \beta_1 G_x(0) = 0 \\ \alpha_2 G(L) + \beta_2 G_x(L) = 0 \end{aligned}$$

Consider the solution for $x < \xi$. The left BC gives

$$G = Ay_1(x)$$

For $x > \xi$, the right BC gives

$$G = By_2(x)$$

The Green's function also has to satisfy: i) $[G]_\xi = G(\xi^+, \xi) - G(\xi^-, \xi) = 0$; ii) $[G_x]_\xi = -1/p(\xi)$, which is found by integrating (1) near $x = \xi$

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

Imposing these restrictions gives

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

where the Wronskian is given by

$$W = y_1 y_2' - y_1' y_2$$

Then u can be expressed as

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