AMATH 568: Homework 3
Winter Quarter 2023
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Due: January 25, 2023

1. *Particle in a box:* Consider the time-dependent Schrodinger 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 Schrodinger 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) Filling in ψ gives us

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

This is the time-independent Schrödinger equation.

(b) Define the operator L as

$$Lu := -\frac{\partial}{\partial x}\left[\frac{\hbar^2}{2m}\frac{\partial u}{\partial x}\right] + V(x)u.$$

We then get that the time-independent Schrödinger equation becomes

$$Lu = Eu,$$

clearly an eigenvalue problem. The operator is also of Sturm-Liouville type since here we have that $p(x) = \frac{\hbar^2}{2m}$ and $q(x) = V(x)$. The boundary conditions are not given.

(c) Say that

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

We then have that the operator is defined for $x \in]-L, L[$ and is

$$Lu = -\frac{\hbar^2}{2m}\frac{\partial^2 u}{\partial x^2}.$$

We thus want to solve the following problem:

$$Lu = Eu, \text{ where } u(L) = u(-L) = 0.$$

The solution to

$$-\frac{\hbar^2}{2m}\frac{\partial^2 u}{\partial x^2} = Eu \Rightarrow \frac{\partial^2 u}{\partial x^2} = -\frac{2Em}{\hbar^2}u$$

is of the form $u(x) = A\cos\left(\frac{\sqrt{2Em}}{\hbar}(x+L)\right) + B\sin\left(\frac{\sqrt{2Em}}{\hbar}(x+L)\right)$. Since $u(-L) = 0$, we have that $A = 0$. Since $u(L) = 0$, we have that $B\sin\left(2\frac{\sqrt{2Em}}{\hbar}L\right) = 0$. As we do not want the trivial solution, we won't take $B = 0$, thus $\sin\left(\frac{2\sqrt{2Em}}{\hbar}L\right) = 0$, therefore $\frac{2\sqrt{2EmL}}{\hbar} = k\pi$, with $k \in \mathbb{N}$. Thus, $E = \frac{1}{8m}\left(\frac{k\pi\hbar}{L}\right)^2$. Because filling in k or $-k$ gives the same result, we will only be taking $k \in \mathbb{Z}$. Later on $\sqrt{k^2}$ will be used, but this is $|k|$, we thus keep it to $\mathbb{Z}$. Since $k = 0$ is the trivial solution, we wont include this: $k \in \mathbb{Z}_0$. Choosing the B comes down to having the eigenfunctions normalized. Therefore:

$$\int_{-L}^{L} B^2 \sin\left(\frac{k\pi}{L}(x+L)\right)^2 dx = 1 \Rightarrow B = \frac{1}{\sqrt{L}},$$

since $\int_0^L \sin\left(\frac{k\pi}{L}x\right)^2 dx = \frac{L}{2}$. Therefore, We have the eigenvalue and normalized eigenfunction pairs:

$$\left(\frac{1}{2m}\left(\frac{k\pi\hbar}{2L}\right)^2, \frac{1}{\sqrt{L}}\sin\left(\frac{k\pi}{L}(x+L)\right)\right).$$

(d) The lowest energy is for $k = 1$ (or $k = -1$), the energy of the ground state E_* is then

$$E_* = \frac{1}{2m}\left(\frac{\pi\hbar}{2L}\right)^2.$$

(e) The energy of the third state E_3 is given by $\dfrac{1}{2m}\left(\frac{3\pi\hbar}{2L}\right)^2$. Therefore, the energy of the electron jumping from the third state to the ground state is

$$E_{jump} = \frac{1}{2m}\left(\frac{\pi\hbar}{2L}\right)^2 - \frac{9}{2m}\left(\frac{\pi\hbar}{2L}\right)^2 = -\frac{1}{m}\left(\frac{\pi\hbar}{L}\right)^2.$$

Since the frequency ω of the emitted photon can be gotten from the energy by $E = \hbar\omega$, therefore we know that

$$\omega_{jump} = \frac{E_{jump}}{\hbar} = -\frac{\hbar}{m}\left(\frac{\pi}{L}\right)^2.$$

(f) If L gets cut in half, we can just replace L by $\frac{L}{2}$. In otherwords, the eigenvalue will multiply by 4 and the amplitude of the eigenfunction will be multiplied by $\sqrt{2}$. Of course the frequency is also going to get higher. We would also not put $(x+L)$ in the eigenfunction, but just x, since a starting point is now just 0. Note that we could have just used $(x-L)$ for both cases. Therefore we get the following eigenvalues and normalized eigenfunctions:

$$\left(\frac{1}{2m}\left(\frac{k\pi\hbar}{L}\right)^2, \sqrt{\frac{2}{L}}\sin\left(\frac{2k\pi}{L}x\right)\right).$$

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

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

Solution:

(a) First we define the operator L :

$$Lu := (u')' + c^2u.$$

Note that we already proved that this is self-adjoint in the last homework set with these boundary conditions: $p(x) = -1,\ q(x) = c^2,\ \alpha_{1/2} = 1$ and $\beta_{1/2} = 0$. Remind yourself that the Green's function is found by

$$L^\dagger G(x,\xi) = \delta(x-\xi),$$

but since L is self-adjoint, we have that

$$LG(x,\xi) = \delta(x-\xi).$$

Define notation

$$[f]_\xi = \lim_{\epsilon\to 0} f(\xi+\epsilon) - f(\xi-\epsilon).$$

Assume that the Green's function is continuous, we then have that $[G]_\xi = 0,\ \forall\xi\ \in]0,L[$. Looking at the integral as calculating the area under the curve, we get that, for $\xi \in]0,L[$ and $\epsilon > 0$ such that $\xi \pm \epsilon \in]0,L[$,

$$\begin{aligned}
\int_{\xi-\epsilon}^{\xi+\epsilon} \delta(x-\xi)dx &= \int_{\xi-\epsilon}^{\xi+\epsilon} LGdx \\
1 &= \int_{\xi-\epsilon}^{\xi+\epsilon} (G')' + c^2Gdx \\
&\overset{\epsilon\to 0}{=} [G']_\xi
\end{aligned}$$

Note that $\int_{\xi-\epsilon}^{\xi+\epsilon} Gdx$ goes to zero since we assume G is continuous and for $\epsilon \to 0$ we get $\int_\xi^\xi Gdx = 0$. Next to the initial boundary conditions, we thus also have the following conditions:

$$[G]_\xi = 0, \text{ and } [G']_\xi = 1.$$

Now we can look at solving the equation

$$LG = \delta(x-\xi),$$

since we have four conditions and are going to get two functions which have to fulfill a second order ODE. Namely, for $x < \xi$:

$$LG = 0 \Rightarrow G'' + c^2G = 0, \text{ with } G(0) = 0,$$

and for $x > \xi$

$$LG = 0 \Rightarrow G'' + c^2G = 0, \text{ with } G(L) = 0.$$

It is easy to see that in both cases G will be the linear combination of a sine and cosine. For $x < \xi$ we get

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

but since $G(0,\xi) = 0$, we have that $A = 0$, thus $G(x,\xi) = B\sin(cx)$. On the other hand for $x > \xi$, we can choose

$$G(x,\xi) = C\cos(c(x-L)) + D\sin(c(x-L)),$$

which, because of $G(L,\xi) = 0$ we have that $C = 0$, gives us that $G(x,\xi) = D\sin(c(x-L))$. Therefore

$$G(x,\xi) = \begin{cases} B\sin(cx) & 0 \le x < \xi \\ D\sin(c(x-L)) & \xi < x \le L \end{cases} = \begin{cases} By_1(x) & 0 \le x < \xi \\ Dy_2(x) & \xi < x \le L \end{cases}.$$

We can get B and D by using the other 2 conditions that we set up. Let's get a more general formula for these solutions. This gives us (dropping the ξ dependence after step one):

$$\begin{cases} Dy_2(\xi) - By_1(\xi) = 0 \\ Dy_2'(\xi) - By_1'(\xi) = 1 \end{cases} \Rightarrow \begin{cases} D = \frac{y_1}{y_2}B \\ \frac{y_1 y_2'}{y_2}B - By_1' = 1 \end{cases}$$

$$\Rightarrow \begin{cases} D = \frac{y_1}{y_2}B \\ (y_1y_2' - y_1'y_2)B = y_2 \end{cases} \Rightarrow \begin{cases} D = \frac{y_1}{y_1y_2' - y_1'y_2} \\ B = \frac{y_2}{y_1y_2' - y_1'y_2} \end{cases}$$

$$\Rightarrow \begin{cases} D = \frac{y_1(\xi)}{W[y_1,y_2](\xi)} \\ B = \frac{y_2(\xi)}{W[y_1,y_2](\xi)} \end{cases}$$

Note that $\xi \neq 0, L$, thus we are not dividing by zero. Therefore, the Green's function is

$$G = \begin{cases} \frac{y_1(x)y_2(\xi)}{W[y_1,y_2](\xi)} & 0 \le x < \xi \\ \frac{y_1(\xi)y_2(x)}{W[y_1,y_2](\xi)} & \xi < x \le L \end{cases}.$$

With W being the Wronskain. Note here that we can simplify the Wronskain here to being:

$$W[y_1, y_2](\xi) = c\sin(c\xi)\cos(c(\xi - L)) - c\cos(c\xi)\sin(c(\xi - L)) = c\sin(cL).$$

Note also that we haven't defined $G(\xi, \xi)$, but since we want it to be continuous, it can easily be defined in the function. However, since we are going to use it only in an integral setting, we don't really need that one x value. Nevertheless, the explicit form of the Green's function is

$$G = \begin{cases} \dfrac{\sin(c(\xi - L))\sin(cx)}{c\sin(cL)} & 0 \le x \le \xi \\ \dfrac{\sin(c\xi)\sin(c(x - L))}{c\sin(cL)} & \xi \le x \le L \end{cases}.$$

Now that we know what the Green's function is, we should be able to find a solution. This as

$$\begin{aligned} f(x) &= Lu \\ \langle f(x), G(x,\xi)\rangle &= \langle Lu, G(x,\xi)\rangle \\ \int_0^L f(x)G(x,\xi)dx &= \langle u, LG(x,\xi)\rangle \\ &= \langle u, \delta(x-\xi)\rangle \\ &= u(\xi) \\ &\Rightarrow \\ u(x) &= \int_0^L f(\xi)G(\xi,x)d\xi \end{aligned}$$

In conclusion, the solution u, in terms of the Green's function, is

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

(b) We can do part (a) over again, a lot is the same, however for the sake of your time, I will do it faster:

The operator L is once again self-adjoint (see previous homework). The only difference with (a) is that $q(x) = -c^2$. We also want the Green's function to be continuous, thus $[G]_\xi = 0$ and condition

$$[G']_\xi = 1,$$

must hold again. The big difference here is that our Green's function has a different general form for $x < \xi$ and $x > \xi$. We have for these cases that

$$G(x,\xi) = \begin{cases} Ae^{cx} + Be^{-cx} & 0 \le x \le \xi \\ Ce^{c(x-L)} + De^{-c(x-L)} & \xi \le x \le L \end{cases}.$$

Because of the boundary conditions, we get that $B = -A$ and $D = -C$. Therefore,

$$G(x,\xi) = \begin{cases} A\left(e^{cx} - e^{-cx}\right) & 0 \le x \le \xi \\ C\left(e^{c(x-L)} - e^{-c(x-L)}\right) & \xi \le x \le L \end{cases} = \begin{cases} Ay_1(x) & 0 \le x \le \xi \\ Cy_2(x) & \xi \le x \le L \end{cases}.$$

Using the same formula as in the previous part (note that we can't divide by $\xi \neq 0, L$), we want to find out what the Wronskian is. This is

$$W[y_1, y_2](\xi) = c\left(e^{c\xi} - e^{-c\xi}\right)\left(e^{c(\xi-L)} + e^{-c(\xi-L)}\right) - c\left(e^{c\xi} + e^{-c\xi}\right)\left(e^{c(\xi-L)} - e^{-c(\xi-L)}\right) = 2c\left(e^{cL} - e^{-cL}\right).$$

In conclusion, the Green's function is given by

$$G(x,\xi) = \begin{cases} \dfrac{\left(e^{c(\xi-L)} - e^{-c(\xi-L)}\right)\left(e^{cx} - e^{-cx}\right)}{2c\left(e^{cL} - e^{-cL}\right)} & 0 \le x \le \xi \\ \dfrac{\left(e^{c\xi} - e^{-c\xi}\right)\left(e^{c(x-L)} - e^{-c(x-L)}\right)}{2c\left(e^{cL} - e^{-cL}\right)} & \xi \le x \le L \end{cases}.$$

The solution $u(x)$ is then given by,

$$u(x) = \int_0^L f(\xi)G(\xi,x)d\xi = \frac{e^{c(x-L)} - e^{-c(x-L)}}{2c\left(e^{cL} - e^{-cL}\right)} \int_0^x f(\xi)\left(e^{c\xi} - e^{-c\xi}\right)d\xi$$
$$+ \frac{e^{cx} - e^{-cx}}{2c\left(e^{cL} - e^{-cL}\right)} \int_x^L f(\xi)\left(e^{c(\xi-L)} - e^{-c(\xi-L)}\right)d\xi$$

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)

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

with

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

Solution:

As seen in the second exercise, we want to find

$$LG = \delta(x - \xi). \tag{1}$$

It's only this equation, since we've already seen that L is self-adjoint (see homework 2). Like exercise 2, we first want to find some more conditions. One of them we lay down on the function ourselves, namely, that the Green's function needs to be continuous for every $\xi \in]0, L[$:

$$[G]_\xi = 0.$$

Another condition can be found by integration of (1) for variable x over $\Xi = [\xi - \epsilon, \xi + \epsilon] \subset [0, L]$:

$$\begin{aligned} \int_\Xi \delta(x-\xi)dx &= \int_\Xi LGdx \\ 1 &= -\int_\Xi [p(x)G_x]_x + \int_\Xi qGdx \\ &\overset{\epsilon \to 0}{=} -[pG_x]_\xi \\ &= -p(\xi)[G_x]_\xi \\ &\Rightarrow \\ [G_x]_\xi &= \frac{-1}{p(\xi)}. \end{aligned}$$

We now have four conditions which the Green's function must satisfy. This is just enough since the L operator uses a derivative of the second order and because of the discontinuity in $x = \xi$, we have that there will be a split in solution. One must thus look at 2 different solutions of the differential equation

$$LG = 0.$$

One of which is for $x < \xi$ and the other for $x > \xi$. Since we have one boundary condition per situation, we can get rid of one of the parameters which will be in the general solution. That is why we can say that the Green's function will be of the form

$$G = \begin{cases} Ay_1(x) & 0 \le x \le \xi \\ By_2(x) & x \le \xi \le L \end{cases}$$

Note that we can say lesser than or equal to because of the continuoutiy condition we demanded. Also assume that neither can be equal to zero.

We now want to use the conditions we "found" in order to find A and B:

$$\begin{aligned} &\begin{cases} By_2(\xi) - Ay_1(\xi) = 0 \\ By_2'(\xi) - Ay_1'(\xi) = \frac{-1}{p(\xi)} \end{cases} &&\Rightarrow \begin{cases} B = \frac{y_1}{y_2}A \\ \frac{y_1 y_2'}{y_2}A - Ay_1' = \frac{-1}{p(\xi)} \end{cases} \\ \Rightarrow &\begin{cases} B = \frac{y_1}{y_2}A \\ (y_1y_2' - y_1'y_2)A = \frac{-y_2}{p(\xi)} \end{cases} &&\Rightarrow \begin{cases} B = \frac{-y_1}{p(\xi)(y_1y_2' - y_1'y_2)} \\ A = \frac{-y_2}{p(\xi)(y_1y_2' - y_1'y_2)} \end{cases} \\ \Rightarrow &\begin{cases} B = \frac{-y_1(\xi)}{p(\xi)W[y_1,y_2](\xi)} \\ A = \frac{-y_2(\xi)}{p(\xi)W[y_1,y_2](\xi)} \end{cases} \end{aligned}$$

Therefore, the Green's function is given by

$$G = \begin{cases} \dfrac{-y_1(x)y_2(\xi)}{p(\xi)W[y_1,y_2](\xi)} & 0 \le x \le \xi \\ \dfrac{-y_1(\xi)y_2(x)}{p(\xi)W[y_1,y_2](\xi)} & \xi \le x \le L \end{cases}$$

Once again, now that we know what the Green's function is, we should be able to find a solution. This as

$$\begin{aligned}
f(x) &= Lu \\
\langle f(x), G(x,\xi)\rangle &= \langle Lu, G(x,\xi)\rangle \\
\int_0^L f(x)G(x,\xi)dx &= \langle u, LG(x,\xi)\rangle \\
&= \langle u, \delta(x-\xi)\rangle \\
&= u(\xi) \\
&\Rightarrow \\
u(x) &= \int_0^L f(\xi)G(\xi,x)d\xi
\end{aligned}$$

In conclusion, the solution to the Stur-Liouville problem using the Green's function approach is,

$$u(x) = \frac{-y_2(x)}{p(x)W[y_1,y_2](x)}\int_0^x f(\xi)y_1(\xi)d\xi - \frac{y_1(x)}{p(x)W[y_1,y_2](x)}\int_x^L f(\xi)y_2(\xi)d\xi.$$

Note that the solutions to exercise 2 fit this formula.