MATH 272, HOMEWORK 9, *Solutions*

Problem 1. Let $\Psi(x)$ be a complex function with domain $[0, L]$. Show that multiplication by a global phase $e^{i\theta}$ does not affect the norm of $\Psi(x)$ under the Hermitian (integral) inner product. In more generality, this shows that you cannot fully determine a quantum state – there will always be an undetermined phase.

Solution 1. We take the following

$$\begin{aligned}
\|e^{i\theta}\Psi\|^2 = \langle e^{i\theta}\Psi, e^{i\theta}\Psi\rangle &= \int_0^L \left(e^{i\theta}\Psi(x)\right)\left(e^{i\theta}\Psi(x)\right)^* dx \\
&= \int_0^L e^{i\theta}e^{-i\theta}\Psi(x)\Psi^*(x)dx \\
&= \int_0^L \Psi(x)\Psi^*(x)dx \\
&= \langle \Psi, \Psi\rangle \\
&= \|\Psi\|^2.
\end{aligned}$$

Problem 2. Consider the real function $f(x) = 1$ on the domain $[0, L]$.

(a) What is the norm of f, $\|f\|$?

(b) Normalize $f(x)$.

(c) Find a nonzero normalized polynomial of degree ≤ 1 that is orthogonal to $f(x)$.

Solution 2.

(a) We compute the norm by

$$\begin{aligned}\|f\| = \sqrt{\langle f, f\rangle} &= \sqrt{\int_0^L f^2(x)dx} \\ &= \sqrt{\int_0^L 1dx} \\ &= \sqrt{L}.\end{aligned}$$

(b) We can normalize f by letting c be some constant and forcing

$$1 = \|cf\| = c^2 L.$$

Thus $c = \frac{1}{\sqrt{L}}$. We can write the normalized function as

$$h(x) = \frac{1}{\sqrt{L}}.$$

(c) Consider an arbitrary polynomial of degree ≤ 1 by putting $g(x) = ax + b$. Now, we want this polynomial to be orthogonal to $f(x)$ which means that we want

$$\langle f, g\rangle = 0.$$

Let us compute the above

$$\begin{aligned}\langle f, g\rangle &= \int_0^L f(x)g(x)dx \\ &= \int_0^L ax + bdx \\ &= \frac{aL^2}{2} + bL \\ &= \frac{1}{2}L\left(aL + 2b\right).\end{aligned}$$

Hence, we can solve for a by

$$0 = aL + 2b \quad \implies \quad a = -\frac{2b}{L}.$$

Now, $g(x) = -\frac{2b}{L}x + b$. But, we require $g(x)$ to be normalized as well hence

$$1 = \langle g, g \rangle = \int_0^L \left(-\frac{2b}{L}x + b \right)^2 dx$$
$$= \frac{b^2 L}{3}.$$

Solving for b, we find $b = \sqrt{\frac{3}{L}}$ and hence we have that

$$g(x) = -2\sqrt{\frac{3}{L^3}}x + \sqrt{\frac{3}{L}}..$$

Problem 3. A wavefunction $\Psi(x)$ for a particle in the 1-dimensional box $[0, L]$ could be written as a superposition of normalized states

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right).$$

That is,

$$\Psi(x) = \sum_{n=1}^{\infty} a_n \psi_n(x),$$

for some choice of the coefficients a_n.

(a) Let $a_n = \frac{\sqrt{6}}{n\pi}$. Show that $\Psi(x)$ is normalized. *Hint: first, use orthogonality of the states $\psi_n(x)$ to your advantage. Then you will need to know what an infinite series evaluates to. Use a tool like WolframAlpha to evaluate this series.*

(b) Note that we can approximate $\Psi(x)$ by taking a finite sum approximation up to some chosen N by

$$\Psi(x) \approx \sum_{n=1}^{N} a_n \psi_n(x).$$

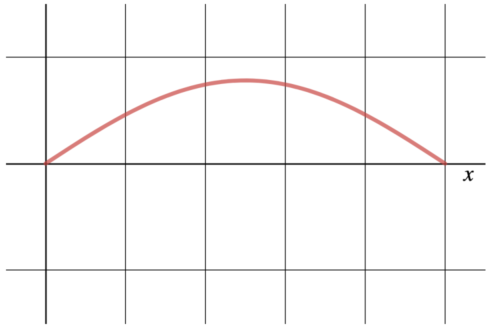
Plot the approximation of $\Psi(x)$ for $N = 1, 5, 50, 100$. *Hint: you can modify my Desmos examples.*

Solution 3. (a) To see that $\Psi(x)$ is normalized we take

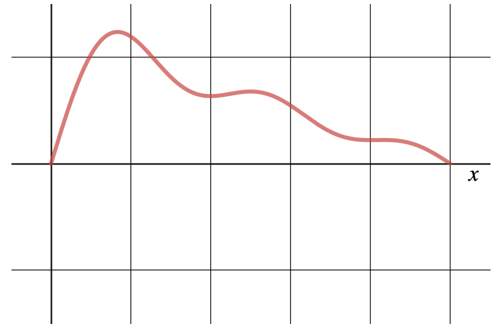
$$\begin{aligned}
\langle \Psi, \Psi \rangle &= \langle \sum_{n=1}^{\infty} a_n \psi_n(x), \sum_{n=1}^{\infty} a_n \psi_n(x) \rangle \\
&= \sum_{n=1}^{\infty} \|a_n\|^2 \langle \psi_n, \psi_n \rangle && \text{by orthogonality of the states} \\
&= \sum_{n=1}^{\infty} \frac{6}{n^2 \pi^2} \\
&= \frac{6}{\pi^2} \sum_{n=1}^{\infty} \frac{1}{n^2} \\
&= \frac{6}{\pi^2} \zeta(2) \\
&= 1.
\end{aligned}$$

Note the sum above is the Zeta function we saw in Math 271 and $\zeta(2)$ is a well-known value (that you can find by computing the above sum in, for example, WolframAlpha.

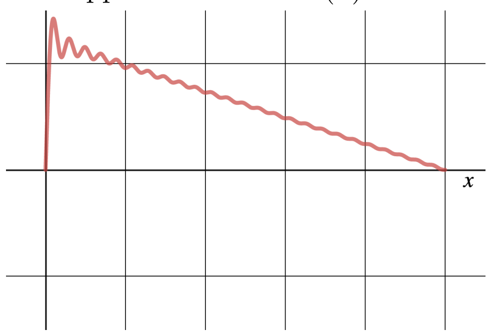
(b)



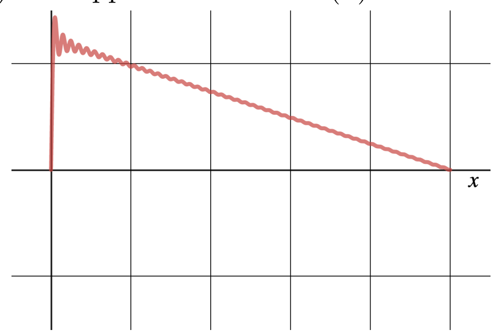
(a) The approximation to $\Psi(x)$ with $N = 1$.



(b) The approximation to $\Psi(x)$ with $N = 5$.



(c) The approximation to $\Psi(x)$ with $N = 50$.



(d) The approximation to $\Psi(x)$ with $N = 100$.

Problem 4. When making a measurement of the position of the particle, we will use the *position operator* x. This is the same as the variable x in the original problem statement, but it is also an operator!

(a) Show that the position operator x is Hermitian.

(b) We can compute the expected position of a particle with wavefunction $\Psi(x)$ by computing

$$\mathbb{E}[x] = \langle \Psi, x\Psi \rangle.$$

Let $\Psi(x) = \frac{1}{\sqrt{2}}\psi_1(x) + \frac{1}{\sqrt{2}}\psi_2(x)$, compute $\mathbb{E}[x]$. This value $\mathbb{E}[x]$ tells you where we expect to find the particle on average.

(c) In fact, any real valued function $V(x)$ of the position operator x is also Hermitian. Make a quick argument on why this must be true.

Solution 4. (a) Let $\Psi(x)$ and $\Phi(x)$ be arbitrary functions. Then we have

$$\begin{aligned}
\langle x\Psi, \Phi \rangle &= \int_0^L x\Psi(x)\Phi^*(x)dx \\
&= \int_0^L \Psi(x)\left(x\Phi(x)\right)^* dx && \text{since } x \text{ is real valued} \\
&= \langle \Psi, x\Phi \rangle.
\end{aligned}$$

Thus we have that the position operator is Hermitian.

(b) We can compute the expected value by

$$\begin{aligned}
\mathbb{E}[x] = \langle \Psi, x\Psi \rangle &= \int_0^L \Psi(x)x^*\Psi(x)dx \\
&= \int_0^L x\left(\frac{1}{\sqrt{2}}\psi_1(x) + \frac{1}{\sqrt{2}}\psi_2(x)\right)^2 dx \\
&= \int_0^L x\left(\frac{1}{2}\psi_1^2(x) + \psi_1(x)\psi_2(x) + \frac{1}{2}\psi_2^2(x)\right) dx.
\end{aligned}$$

This can be split into three separate integrals. First,

$$\int_0^L \frac{x}{2}\psi_1^2(x)dx = \int_0^L \frac{x}{L}\sin^2\left(\frac{\pi x}{L}\right)dx = \frac{L}{4}.$$

Second,

$$\int_0^L x\psi_1(x)\psi_2(x)dx = \int_0^L \frac{2x}{L}\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi x}{L}\right)dx = -\frac{16L}{9\pi^2}.$$

Finally,

$$\int_0^L x\psi_2^2(x)dx = \int_0^L \frac{x}{L}\sin^2\left(\frac{2\pi x}{L}\right)dx = \frac{L}{4}.$$

Thus, we can add these all together to get

$$\boxed{\mathbb{E}[x] = \frac{L}{2} - \frac{16L}{9\pi^2} \approx .32L}.$$

(c) If $V(x)$ is real valued, then $V^*(x) = V(x)$. Hence, we have

$$\langle V\Psi, \Phi\rangle = \int_0^L V(x)\Psi(x)\Phi^*(x)dx = \int_0^L \Psi(x)\left(V(x)\Phi(x)\right)^* dx = \langle \Psi, V\Phi\rangle.$$

Problem 5. Another related operator is the *momentum operator* $p = -i\hbar\frac{d}{dx}$. Using integration by parts, show that this operator is Hermitian.

Solution 5. We have

$$\begin{aligned}\langle p\Psi, \Phi\rangle &= \int_0^L \left(-i\hbar\frac{d\Psi}{dx}\right)\Phi^*(x)dx \\ &= -i\hbar\Psi(x)\Phi^*(x)\big|_0^L + \int_0^L i\hbar\Psi(x)\frac{d\Phi^*}{dx}dx \qquad \text{by integration by parts.}\end{aligned}$$

Note now that the boundary conditions require both $\Psi(0) = \Psi(L) = 0$ and $\Phi(0) = \Phi(L) = 0$, since we are working over the space of solutions to the particle in the 1-dimensional box. Hence, we have

$$\begin{aligned}\langle p\Psi, \Phi\rangle &= \int_0^L i\hbar\Psi(x)\frac{d\Phi^*}{dx}dx \\ &= \int_0^L \Psi(x)\left(-i\hbar\frac{d\Phi}{dx}\right)^* dx \\ &= \langle \Psi, p\Phi\rangle.\end{aligned}$$

Thus, p is Hermitian.

Problem 6. We can always take products, sums, and scalar multiples of operators to build new operators. For example, in classical physics, we have the kinetic energy

$$T = \frac{1}{2} m \vec{\boldsymbol{v}} \cdot \vec{\boldsymbol{v}},$$

where $\vec{\boldsymbol{v}}$ is the velocity. In 1-dimension, this reduces to the familiar $\frac{1}{2}mv^2$. However, we can also rewrite this 1-dimensional equation using the momentum $p = mv$ which gives us the kinetic energy

$$T = \frac{p^2}{2m}.$$

Hence, we can define the quantum *kinetic energy operator*

$$T = \frac{p^2}{2m}.$$

(a) Show that $T = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2}$.

(b) Make a quick argument as to why this kinetic energy operator T is Hermitian.

(c) Again, letting $\Psi(x) = \frac{1}{\sqrt{2}}\psi_1(x) + \frac{1}{\sqrt{2}}\psi_2(x)$, compute $\mathbb{E}[T]$. The expected value $\mathbb{E}[T]$ tells us what the observed energy will be on average. Yet, any time we measure a system we will find that energy must be one of the energy eigenvalues. Thus, for this wave function, this expected value should be the average between E_1 and E_2 which means that half the time we will measure the energy to be E_1 and half the time it will be E_2.

Solution 6.

(a) We have $p = -i\hbar\frac{d}{dx}$. Then, we construct T by

$$\begin{aligned} T = \frac{p^2}{2m} &= \frac{\left(-i\hbar\frac{d}{dx}\right)^2}{2m} \\ &= \frac{-\hbar^2}{2m}\frac{d^2}{dx^2}. \end{aligned}$$

(b) We have

$$\begin{aligned} \langle T\Psi, \Phi\rangle &= \langle \frac{p^2}{2m}\Psi, \Phi\rangle \\ &= \langle p^2\Psi, \frac{1}{2m}\Phi\rangle && \text{since } \frac{1}{2m} \text{ is a real constant} \\ &= \langle p\Psi, \frac{p}{2m}\Phi\rangle && \text{since } p \text{ is Hermitian} \\ &= \langle \Psi, \frac{p^2}{2m}\Phi\rangle \\ &= \langle \Psi, T\Phi\rangle. \end{aligned}$$

Thus, T is Hermitian.

(c) Now, most of the work has been done for us, and the rest here will be taken care of by orthogonality. We take

$$\begin{aligned}
\langle \Psi, T\Psi \rangle &= \langle \frac{1}{\sqrt{2}}\psi_1 + \frac{1}{\sqrt{2}}\psi_2, \frac{E_1}{\sqrt{2}}\psi_1 + \frac{E_2}{\sqrt{2}}\psi_2 \rangle \\
&= \frac{E_1}{2}\langle \psi_1, \psi_1 \rangle + \frac{E_1}{2}\langle \psi_2, \psi_1 \rangle + \frac{E_2}{2}\langle \psi_1, \psi_2 \rangle + \frac{E_2}{2}\langle \psi_2, \psi_2 \rangle \\
&= \frac{E_1 + E_2}{2}.
\end{aligned}$$

Problem 7. If we are given a potential (energy) $V(x)$ and the kinetic energy T, we can take their sum and form the total energy $T + V(x)$ which we call the *Hamiltonian.* Thus, in the quantum realm, we create the Hamiltonian operator H by

$$H = T + V(x).$$

(a) Show that the Hamiltonian operator is Hermitian. *Hint: you have already done the necessary work for this. You just need to combine it and show a few steps here.*

(b) The spectrum of the Hamiltonian tells us the possible energy eigenvalues of a quantum system. Thus, we can compute the spectrum (in this case) by solving the eigenvalue equation

$$H\Psi(x) = E\Psi(x).$$

Explain why the spectrum of H is discrete for the particle in the box problem. *Hint: We have done this exact problem in the notes from Math 271. Feel free to use that!*

Solution 7. (a) We know that both T and $V(x)$ are Hermitian. Thus, we take

$$\langle (T+V)\Psi, \Phi\rangle = \langle T\Psi, \Phi\rangle + \langle V\Psi, \Phi\rangle = \langle \Psi, T\Phi\rangle + \langle \Psi, V\Phi\rangle = \langle \Psi, (T+V)\Phi\rangle$$

(b) Since $V(x) = 0$ in $[0, L]$, we have that

$$H = T = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}.$$

Hence, we are solving the equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\Psi(x) = E\Psi(x).$$

Let $\omega^2 = \frac{2mE}{\hbar^2}$, and we have

$$\Psi''(x) + \omega^2\Psi(x) = 0,$$

which is the harmonic oscillator equation. Thus, our solution is

$$\Psi(x) = C_1e^{i\omega x} + C_2e^{-i\omega x}.$$

Now, if we apply the boundary conditions, we have

$$0 = \Psi(0) = C_1 + C_2,$$

thus $C_1 = -C_2$. By Euler's formula, we can take

$$C_1e^{i\omega x} - C_1e^{-i\omega x} = C\sin(\omega x).$$

Now, our other boundary condition states

$$0 = \Psi(L) = C\sin(\omega L),$$

Thus we must have $\omega = \frac{n\pi}{L}$ for an integer n. Now, this means

$$\frac{2mE}{\hbar^2} = \omega^2 = \frac{n^2\pi^2}{L^2},$$

and we can solve for E to get

$$\boxed{E = \frac{n^2\pi^2\hbar^2}{2mL^2},}$$

which shows that the spectrum of H is discrete.