HW 3

Let's solve Schrödinger's equation for a particle on $\mathbb{R}$ with different potential functions. First let's recall some context for quantum mechanics on the real line.

Definition 1.

Let $\mathcal{H}$ be a Hilbert space. An *unbounded operator* on $\mathcal{H}$ is a pair $(L, \mathrm{Dom}(L))$, where $\mathrm{Dom}(L)$ is a dense subspace of $\mathcal{H}$ and

$$L : \mathrm{Dom}(L) \to \mathcal{H}$$

is a linear map.

Bounded operators are a special case of unbounded operators, for which $\mathrm{Dom}(L) = \mathcal{H}$. (So a better name for unbounded operators might be "not necessarily bounded operators", but we choose the shorter name for obvious reasons.) It will be convenient to have some nice dense subspaces of $L^2(\mathbb{R})$ on hand for later.

Theorem 2.

The following are dense subspaces of $L^2(\mathbb{R})$.

(i) The space of compactly supported simple functions

$$\mathrm{Sim}_c(\mathbb{R}) = \mathrm{span}\{\, \mathbb{1}_E \mid E \subseteq \mathbb{R} \text{ is compact} \,\}.$$

(ii) The space of smooth compactly supported functions

$$C_c^\infty(\mathbb{R}) = \{f \in C^\infty(\mathbb{R}, \mathbb{C}) \mid f \text{ has compact support}\}.$$

A function $f : \mathbb{R} \to \mathbb{C}$ has *compact support* if there is some $R > 0$ such that $f(x) = 0$ whenever $|x| > R$.

Just like with bounded normal operators, unbounded normal operators can be diagonalized. We need to expand our notion of diagonal operators, however, to allow for the unbounded case.

Definition 3.

Let X be a measure space. If $f : X \to \mathbb{C}$ is a measurable function, then we define an unbounded operator L_f on $L^2(X)$ via

$$L_f(\psi) \doteq f\psi$$

for any ψ in the set

$$\mathrm{Dom}(L_f) \doteq \{\, \psi \in L^2(X) \mid f\psi \in L^2(X) \,\}.$$

If L is an unbounded operator on $L^2(X)$, then we say L is *diagonal* (or *multiplicative*) if there is some measurable $f : X \to \mathbb{C}$ such that $L = L_f$. (Note that equality of unbounded operators entails equality of their domains.)

If L_f is any diagonal operator on $L^2(X)$ and $g : \mathbb{C} \to \mathbb{C}$ is a measurable function, then we define

$$g(L_f) \doteq L_{g \circ f}.$$

This procedure is called the *Borel functional calculus*. In general we only need g to be defined on the range of f.

A diagonal operator $L = L_f$ is bounded if and only if the function $f : X \to \mathbb{C}$ is essentially bounded. There are two important unbounded operators on $L^2(\mathbb{R})$ for quantum mechanics.

Definition 4.

Let $\widehat{X}$ be the unbounded diagonal operator on $L^2(\mathbb{R})$ defined by

$$\widehat{X} \doteq L_{\mathrm{id}_{\mathbb{R}}},$$

where $\mathrm{id}_{\mathbb{R}} : \mathbb{R} \to \mathbb{C}$ is the measurable function defined by

$$\mathrm{id}_{\mathbb{R}}(x) = x.$$

$\widehat{X}$ is called the *position operator* on $L^2(\mathbb{R})$.

The *momentum operator* on $L^2(\mathbb{R})$ is the operator $\widehat{P}$ defined on $C_c^\infty(\mathbb{R})$ by

$$\widehat{P}(\psi) = -i\hbar \frac{d\psi}{dx}.$$

Here $\hbar$ is a physical constant approximately equal to

$$1.055 \times 10^{-34} \ \mathrm{kg} \frac{\mathrm{m}^2}{\mathrm{s}}.$$

We will take the domain of $\widehat{P}$ to actually be much larger than $C_c^\infty(\mathbb{R})$, though; we postpone defining it fully until later.

It turns out that the momentum operator is diagonalizable. To put this in the more general context using the spectral theorem, we need to define what it means for an unbounded operator to be normal.

Definition 5.

Let $\mathcal{H}_1, \mathcal{H}_2$ be Hilbert spaces, and let $\mathrm{Dom}(L) \subseteq \mathcal{H}_1$ be a dense subspace. Let $L : \mathrm{Dom}(L) \to \mathcal{H}_2$ be a linear map. We will define the *adjoint* of L to be a partially defined map $\mathcal{H}_2 \to \mathcal{H}_1$ as follows. We set

$$\mathrm{Dom}(L^*) \doteq \{\, \mathbf{v} \in \mathcal{H}_2 \mid \exists! \mathbf{u} \in \mathcal{H}_1, \ \langle \mathbf{u}, \mathbf{w} \rangle = \langle \mathbf{v}, L\mathbf{w} \rangle \ \text{ for all } \mathbf{w} \in \mathrm{Dom}(L) \,\}.$$

Then the adjoint of L is the unique linear map $L^* : \mathrm{Dom}(L^*) \to \mathcal{H}_1$ such that

$$\langle L^*\mathbf{v}, \mathbf{w}\rangle = \langle \mathbf{v}, L\mathbf{w}\rangle$$

for all $\mathbf{v} \in \mathrm{Dom}(L^*)$ and $\mathbf{w} \in \mathrm{Dom}(L)$.

A (non-trivially) equivalent description of the domain of L^* is

$$\mathrm{Dom}(L^*) = \{\, \mathbf{v} \in \mathcal{H}_2 \mid \text{The map } \mathbf{w} \mapsto \langle \mathbf{v}, L\mathbf{w}\rangle \text{ is a bounded linear map } \mathrm{Dom}(L) \to \mathbb{C} \,\}.$$

In particular, this defines an adjoint map to an unbounded operator L on a Hilbert space. Note, however, that L^* might not have a dense domain, so by our definition it might fail to be an unbounded operator. If this happens, then L^{**} is not well-defined (since density of $\mathrm{Dom}(L)$ is required to define L^*). In all of our cases of interest, however, adjoints will continue to be operators. An operator L for which $\mathrm{Dom}(L^*)$ is dense in $\mathcal{H}$ is said to be a *closeable operator*. We often conflate a closeable operator L with its *closure* $\overline{L}$, defined to be its double adjoint L^{**}. We can now finish defining the momentum operator $\widehat{P}$; it is the closure of the operator $-i\hbar\frac{d}{dx}$ defined above.

To motivate this "closure" terminology, consider the graph of L:

$$\mathrm{Graph}(L) \doteq \{\, (\mathbf{v}, L\mathbf{v}) \in \mathcal{H} \times \mathcal{H} \mid \mathbf{v} \in \mathrm{Dom}(L) \,\}.$$

If L is closeable, then $\mathrm{Graph}(\overline{L})$ is the closure of the set $\mathrm{Graph}(L)$ in $\mathcal{H} \times \mathcal{H}$. The operator L is closeable if and only if $\overline{\mathrm{Graph}(L)}$ is in fact the graph of a partially-defined function. (So L fails to be closeable iff there are distinct $\mathbf{w}_1, \mathbf{w}_2 \in \mathcal{H}$ such that $(\mathbf{v}, \mathbf{w}_1)$ and $(\mathbf{v}, \mathbf{w}_2)$ are both in $\overline{\mathrm{Graph}(L)}$.) From this interpretation, it is clear that $\mathrm{Dom}(\overline{L}) \supseteq \mathrm{Dom}(L)$ and that $\overline{L}$ coincides with L when restricted to $\mathrm{Dom}(L)$.

Theorem 6: Bounded Linear Transformation (BLT) theorem + Closed graph theorem.

Let $\mathrm{Dom}(L)$ be a dense subspace of a Hilbert space $\mathcal{H}$ and let $L : \mathrm{Dom}(L) \to \mathcal{H}$ be a bounded linear map. Then L is a closeable unbounded operator, $\mathrm{Dom}(\overline{L}) = \mathcal{H}$, and $\overline{L}$ is the unique bounded linear operator on $\mathcal{H}$ which restricts to L on $\mathrm{Dom}(L)$.
Conversely, if L is a closeable unbounded operator and $\mathrm{Dom}(\overline{L}) = \mathcal{H}$, then L is a bounded linear map.

So, in a horrible juxtaposition of terms: a bounded operator on a Hilbert space is equivalently a closed unbounded operator which is a bounded linear map.

Definition 7.

Let L be an unbounded operator on a Hilbert space $\mathcal{H}$. We say L is *closed* if L is closeable and $\overline{L} = L$.
We say L is *normal* if the following conditions hold:

(i) $\mathrm{Dom}(L) = \mathrm{Dom}(L^*)$

(ii) $\langle L\mathbf{v}, L\mathbf{w}\rangle = \langle L^*\mathbf{v}, L^*\mathbf{w}\rangle$ for all $\mathbf{v}, \mathbf{w} \in \mathrm{Dom}(L)$.

Equivalently, L is normal if it satisfies the following.

(i') L is closed.

(ii') $\mathrm{Dom}(L^*L) = \mathrm{Dom}(LL^*)$ and $L^*L = LL^*$.

We say L is *self-adjoint* if $L = L^*$.

We say L is *essentially normal* (respectively, *essentially self-adjoint*) if L is closeable and $\overline{L}$ is normal (respectively, self-adjoint). In this case, $\overline{L}$ is the unique extension of L to a normal operator on a larger domain.

Problem 1. o

Let's see how these concepts interact with our diagonal operators. Let $f : \mathbb{R} \to \mathbb{C}$ be a measurable function.

(a) Show that $\mathrm{Dom}((L_f)^*) = \mathrm{Dom}(L_f)$ and that $(L_f)^* = L_{f^*}$. Conclude that L_f is closed.

(b) Show that L_f is normal. If f is real-valued, show that L_f is self-adjoint.

(c) Assume f is real-valued and bounded below. Let L be the restriction of L_f to a dense subspace of $\mathrm{Dom}(L_f)$. Show that L_f is the unique diagonal extension of L. (Note however, that there could be other *diagonalizable* extensions of L, so L could fail to be essentially normal!)

Theorem 8: Spectral theorem for unbounded operators.

Let L be an unbounded operator on a Hilbert space $\mathcal{H}$. Then L is normal if and only if L is *unitarily diagonalizable*: that is, there is a measure space X and a unitary map

$$U : \mathcal{H} \to L^2(X)$$

such that ULU^{-1} is an unbounded diagonal operator on $L^2(X)$.

As a result, the *Borel functional calculus* from Definition 3 can be applied to any unbounded normal operator.

Remark 9. Sadly, there is in general no way to simultaneously diagonalize two unbounded normal operators which commute. The condition that $AB = BA$ must be replaced with the requirement that A and B *strongly commute*, which has no nice equational criterion (at least, without first applying some version of the spectral theorem). Commuting bounded operators always strongly commute.

Let's recall the Fourier transform for $L^2(\mathbb{R})$, which is an application of the spectral theorem for commuting families of bounded operators. In the following, we will make the transform more explicit than we did in class by identifying $\widehat{\mathbb{R}}$ with $\mathbb{R}$. We do so by letting $p \in \mathbb{R}$ correspond to the homomorphism

$$\chi_p : \mathbb{R} \to U(1)$$

$$x \mapsto \exp(\frac{ipx}{\hbar})$$

This allows us to remove explicit mention of $\widehat{\mathbb{R}}$ or χ_p in the description of the Fourier transform.

Theorem 10: Fourier transform.

There is a unique unitary operator

$$\mathcal{F} : L^2(\mathbb{R}) \to L^2(\mathbb{R}),$$

called the *Fourier transform*, which satisfies

$$(\mathcal{F}\psi)(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{\mathbb{R}} \exp(-\frac{ipx}{\hbar})\psi(x)\ dx$$

for all $\psi \in L^2(\mathbb{R}) \cap L^1(\mathbb{R})$.

For each $g \in \mathbb{R}$, let $T_g : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ be the unitary operator defined by

$$T_g(\psi)(x) = \psi(x+g)$$

for $\psi \in L^2(\mathbb{R})$ and $p \in \mathbb{R}$. Then $\mathcal{F}$ is the unique unitary operator (up to scalar multiples) satisfying

$$\mathcal{F}(T_g\psi)(p) = \exp(\frac{ipg}{\hbar})(\mathcal{F}\psi)(p)$$

for all $x, p \in \mathbb{R}$ and $\psi \in L^2(\mathbb{R})$. Up to measurable reparametrizations of $\mathbb{R}$, $\mathcal{F}$ is also the unique unitary operator which simultaneously diagonalizes the collection $\{T_g \mid g \in \mathbb{R}\}$.

If $\widetilde{\psi}$ is in $L^2(\mathbb{R}) \cap L^1(\mathbb{R})$, then

$$(\mathcal{F}^{-1}\widetilde{\psi})(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{\mathbb{R}} \exp(\frac{ipx}{\hbar})\widetilde{\psi}(p)dp.$$

Rather than writing $\mathcal{F}\psi$ for the Fourier transform every time, we often write $\widetilde{\psi}$ instead. Where the function ψ can be thought of as living in the "position basis" (i.e. it is a function of position x), the function $\widetilde{\psi}$ lives in the "momentum basis" (it is a function of momentum p).
Let's explore the relationship between the momentum operator and the Fourier transform. It will turn out that the momentum operator is self-adjoint. Let's see how we can prove this directly first, and then we will apply the Fourier transform to give an easier proof. The following lemma gives a useful criterion for showing that the closure of an operator is self-adjoint.

Lemma 11.

An unbounded operator L on a Hilbert space $\mathcal{H}$ is essentially self-adjoint if

(i) $\langle L\mathbf{v}, \mathbf{w}\rangle = \langle \mathbf{v}, L\mathbf{w}\rangle$ for all $\mathbf{v}, \mathbf{w} \in \mathrm{Dom}(L)$, and

(ii) The image of $L + iI$ is dense in $\mathcal{H}$, and

(iii) The image of $L - iI$ is dense in $\mathcal{H}$.

If L is essentially self-adjoint, then $\overline{L}$ is the unique extension of L to a self-adjoint operator.

Problem 2.

Show, using the previous lemma, that the operator $\widehat{P}_0 = -i\hbar\frac{d}{dx}$ with $\mathrm{Dom}(\widehat{P}_0) \doteq C_c^\infty(\mathbb{R})$ is an essentially self-adjoint operator. You shouldn't need any theorems on differential equations. (You can solve the relevant ones explicitly, though in an abstract way.)

An alternative route to showing that $-i\hbar\frac{d}{dx}$ is essentially self-adjoint is to find a unitary diagonalization for it (or more precisely, for its closure). Conveniently, we already have a unitary map available which will do the deed.

Proposition 12.

Let $\widehat{P}$ be the momentum operator on $L^2(\mathbb{R})$, defined as the closure of $-i\hbar\frac{d}{dx}$ acting on $C_c^\infty(\mathbb{R})$. Then the Fourier transform diagonalizes $\widehat{P}$, and $\mathcal{F}\widehat{P}\mathcal{F}^{-1}$ acts via multiplication by $\mathrm{id}_{\mathbb{R}}$.

Proof. It is equivalent to show that

$$\mathcal{F}(\widehat{P}\psi)(p) = p(\mathcal{F}\psi)(p)$$

for any $\psi \in L^2(\mathbb{R})$ and (almost every) $p \in \mathbb{R}$. In fact, we claim it is sufficient to show this equality just for $\psi \in C_c^\infty(\mathbb{R})$. If we can show the equality for such ψ, then that tells us that $\mathcal{F}\widehat{P}\mathcal{F}^{-1}$ coincides with $L_{\mathrm{id}_{\mathbb{R}}}$ on the space $\mathcal{F}(C_c^\infty(\mathbb{R}))$. This is a dense subspace of $L^2(\mathbb{R})$ by Theorem 2 (and the fact that unitary operators preserve dense subspaces), so by Problem 1(c) the closure of $\mathcal{F}\widehat{P}|_{C_c^\infty(\mathbb{R})}\mathcal{F}^{-1}$ is exactly $L_{\mathrm{id}_{\mathbb{R}}}$. Since $\widehat{P}$ is the closure of $\widehat{P}|_{C_c^\infty(\mathbb{R})}$ (and since unitary maps preserve operator closures), we find that $\mathcal{F}\widehat{P}\mathcal{F}^{-1} = L_{\mathrm{id}_{\mathbb{R}}}$ as desired.

It remains to show that

$$\mathcal{F}(\widehat{P}\psi)(p) = p(\mathcal{F}\psi)(p)$$

for $\psi \in C_c^\infty(\mathbb{R})$. In this case, by definition, we have that

$$\widehat{P}\psi = -i\hbar\psi'.$$

Since any continuous function with compact support is in $L^2(\mathbb{R}) \cap L^1(\mathbb{R})$, we can use the explicit form of the Fourier transform. Thus, we wish to show that

$$\int_{\mathbb{R}} \exp(-\frac{ipx}{\hbar})(-i\hbar\psi'(x))\ dx = p\int_{\mathbb{R}} \exp(-\frac{ipx}{\hbar})\psi(x)\ dx.$$

This equality follows immediately from integration by parts, since

$$\int_{\mathbb{R}} \frac{d}{dx}\left(e^{-\frac{ipx}{\hbar}}\psi(x)\right) dx = 0.$$

□

As a result of the proposition, the momentum operator we defined here in terms of differentiation coincides with the momentum operator we defined in class via the Fourier transform.

Problem 3.

Prove that $\exp(\frac{ig}{\hbar}\hat{P}) = T_g$ for all $g \in \mathbb{R}$, where the exponential is defined using the Borel functional calculus.
Because of this property, we say that *momentum is the infinitesimal generator of translations.*

Now let's use everything so far to do some physics. If L_1, L_2 are two closeable unbounded operators on a Hilbert space then we write $L_1 \simeq L_2$ to indicate that L_1 and L_2 have the same closure. In all of the following you do not need to show work for computational examples (though you are welcome to).

Problem 4: The free Hamiltonian.

Fix a mass $m > 0$. Let $\widehat{H}$ be the unbounded operator on $L^2(\mathbb{R})$ equal to (the closure of)

$$\frac{1}{2m}\widehat{P}^2 \simeq -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}.$$

$\widehat{H}$ is called the *free Hamiltonian.*

(a) Use the Fourier transform to diagonalize $\widehat{H}$. Describe its action as a multiplicative operator in the momentum basis.

(b) Let $\psi_0 \in L^2(\mathbb{R})$. For $t \in \mathbb{R}$, define $\psi_t \in L^2(\mathbb{R})$ via

$$|\psi_t\rangle = U(t)\,|\psi_0\rangle\,,$$

where the time evolution operator $U(t)$ is defined using the Borel functional calculus by

$$U(t) \doteq \exp(-\frac{it}{\hbar}\widehat{H}).$$

Assuming $\psi_0, \widetilde{\psi}_0$ are both integrable (i.e. in $L^1(\mathbb{R})$), use the Fourier transform to write an explicit formula for $\psi_t(x)$.

(c) Specialize part (b) to the Gaussian wavepacket

$$\psi_0(x) = \exp(-x^2).$$

Determine $\psi_t(x)$.

Given an operator L on a Hilbert space, and a nonzero vector $\mathbf{v}$ in $\mathrm{Dom}(L)$, we define the *expectation value* of L on $\mathbf{v}$ to be

$$\langle L \rangle \doteq \frac{\langle \mathbf{v} \mid L\mathbf{v} \rangle}{\langle \mathbf{v} \mid \mathbf{v} \rangle}.$$

(d) Compute $\langle \hat{X} \rangle$ and $\langle \hat{X}^2 \rangle$ for the state ψ_t in part (c).

The free Hamiltonian describes the time evolution for a particle of mass m placed in a vacuum with no external forces acting upon it. In part (d) we found how time evolution affects where we might find that particle. $\langle \widehat{X} \rangle$ measures where we will find the particle on average, whereas $\langle \widehat{X}^2 \rangle$ measures (the square of) how far away from the origin we will expect to find the particle on average.

(e) If you're curious how a state will evolve if it has initial momentum, here is a state with $\langle \widehat{X} \rangle = x_0$ and $\langle \widehat{P} \rangle = p_0$.

$$\psi_0(x) = \exp(-\frac{(x-x_0)^2}{\sigma^2} + i\frac{p_0 x}{\hbar}).$$

There is a variation on the "free particle" quantum system which is also of great importance. This is the "free particle confined to an interval" system, known more commonly as the "particle in an infinite square well".

Problem 5: Infinite square well.

In this quantum system, we take our Hilbert space to be $L^2([0,1])$. This corresponds to restricting our particle to appear only in the interval $[0,1]$. We continue to use the free Hamiltonian $\widehat{H}$, defined as the closure of

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

(now interpreted as an operator on $C_c^\infty([0,1])$).
Physicists interpret this system as a particle living on the real line, with Hamiltonian defined (informally) as

$$\widehat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_{sq}(x),$$

where the infinite square well potential function V_{sq} is

$$V_{sq}(x) = \begin{cases} 0 & \text{if } x \in [0,1] \\ \infty & \text{if } x \notin [0,1] \end{cases}.$$

The domain of this Hamiltonian is, however, not dense in $L^2(\mathbb{R})$, but is instead dense in $L^2([0,1])$, where it coincides (up to closure) with the operator above. (So we may forget that it was originally defined on all of $\mathbb{R}$.)

(a) Find the eigenvalues and eigenspaces of $\widehat{H}$.

(b) Show that the eigenspaces of $\widehat{H}$ give an orthogonal decomposition of $L^2([0,1])$.

(c) Use (b) to describe what the spectrum of $\widehat{H}$ must be.

(d) Diagonalize $\widehat{H}$. Describe the time evolution of a state ψ_0 with appropriate conditions allowing for explicit formulae.

(e) Find the time evolution of some state with interesting behavior. Compute $\langle \widehat{X} \rangle$ and $\langle \widehat{P} \rangle$. Can you find one for which these two expectations oscillate? Give some intuition for why a classical particle might have this behavior.

Problems (b)-(d) may be changed later to give proofs in a more general context (that don't require Fourier series to already be studied).

Now that we've explored what happens to a particle in the absence of forces, let's see what happens when we subject particles to a force. In (basic) quantum mechanics, forces are implemented via a potential function $V : \mathbb{R} \to \mathbb{R}$. Classically, a particle dropped at a point on the real line will try to move towards points with smaller values of the potential. In quantum mechanics, this is also the most probable behavior for a quantum particle (although it also has a chance of doing other things).

More to come in the future!