Next, we seek to identify the <u>momentum operator</u>. The answer will be $P = -i\hbar \frac{\partial}{\partial x}$ (that is, $P_j = -i\hbar \frac{\partial}{\partial x_j}$, $j = 1, \dots, d$). In order to motivate it, we need to consider the group of translations. Let $d=1$ for simplicity. For $a \in \mathbb{R}$, let $T_a : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ be the translation operator:

$$(T_a f)(x) = f(x-a).$$

Then T_a is unitary and it satisfies the group property $T_a T_b = T_{a+b}$ $\forall a, b \in \mathbb{R}$. By Stone theorem there exists a self-adjoint operator P s.t.

$$T_a = e^{-iaP}.$$

Recall Noether's theorem of Hamiltonian Mechanic: to each symmetry corresponds a conserved quantity. For translation invariance, it is momentum. Thus P is the momentum operator.

Further, if f is an analytic function, we have the Taylor series

$$f(x-a) = \sum_{n \geq 0} \frac{(-a)^n}{n!} \frac{d^n}{dx^n} f(x) \text{ " }=\text{ " } e^{-a \frac{d}{dx}} f(x).$$

Then $P = -i \frac{d}{dx}$. For $d \geq 1$, and including physical constants, the momentum operator is $P = -i\hbar \frac{\partial}{\partial x}$.

<u>Exercise 5:</u> Show that P, with $D(P) = L^2 \cap C^1$, is symmetric.

The <u>energy</u> of the system should be given by the operator

$$H = \frac{1}{2m} P^2 + V = -\frac{\hbar^2}{2m} \Delta + V.$$

The evolution should be given by a map $U_t : \psi(0) \mapsto \psi(t)$, assuming determinism. U_t should be linear by the principle of superposition. If the external potential does not change in time, it should satisfy the (semi-)group property $U_s U_t = U_{s+t}$. By Stone's theorem, there exists $\tilde{H}$, self-adjoint, such that $U_t = e^{-it\tilde{H}}$. Time-invariance of the ~~equation~~ laws of motion is a symmetry, and Noether's theorem claims that the energy is conserved. This suggests that $\tilde{H}$ is the energy. We obtain Schrödinger's equation, $i\hbar \frac{\partial}{\partial t} \psi = \left(-\frac{\hbar^2}{2m} \Delta + V\right) \psi$!

A similar reasoning applies to rotations: the operator $X \wedge P$ (or $\vec{X} \times \vec{P}$) is the generator of the unitary group of rotations, and it therefore represents the <u>angular momentum</u>.

3.3 <u>Evolution and Hamiltonian</u>

There are several interesting consequences to the existence of the evolution operator $U_t = e^{-itH}$. If $\psi(0)$ is eigenvector of H with eigenvalue λ, then

$$\psi(t) = e^{-it\lambda} \psi(0).$$

This describes a stationary solution, where $\langle A \rangle_{\psi(t)} = (\psi(t), A\psi(t))$ is constant for all observables A.

Exercise 6. If $H\psi = \lambda\psi$, prove rigorously that $e^{-itH}\psi = e^{-it\lambda}\psi$.

Hints: Show that (i) $(H-ia)^{-1}\psi = (\lambda - ia)^{-1}\psi$, and (ii) $e^{-itH_a}\psi = \exp\{-it\frac{\lambda}{1+\frac{\lambda}{a}}\}\psi$, where H_a is Yosida's approximation.

It is possible to derive an ordinary differential equation for the evolution of observables: If $\psi(t) = e^{-itH}\psi(0)$ is solution to the Schrödinger equation, then

$$\frac{d}{dt}\langle A\rangle_{\psi(t)} = \frac{d}{dt}(U_t\psi(0), AU_t\psi(0)) = \frac{d}{dt}(\psi(0), U_t^* A U_t \psi(0))$$

$$= (\psi(0), \frac{d}{dt} U_t^* A U_t \psi(0)).$$

Recall that $\frac{d}{dt}U_t = -iHU_t$. Then

$$\frac{d}{dt} U_t^* A U_t = iU_t^* HAU_t - iU_t^* AHU_t$$

$$= iU_t^*[H,A]U_t.$$

We find $$\frac{d}{dt}\langle A\rangle_{\psi(t)} = \langle i[H,A]\rangle_{\psi(t)}.$$

This is <u>Heisenberg dynamics</u> of observables. Notice that $\langle A\rangle_{\psi(t)}$ is constant when $\psi(0)$ is eigenvector of H, or when $[H,A]=0$. In particular, energy is conserved, and momentum is conserved in the free evolution ($V=0$, i.e., $H=-\Delta$).

4. THREE EXPLICIT CASES

Exact solutions are useful and much of our intuition on Schrödinger operators is based on them. We seek the spectrum and eigenvectors of $H = -\Delta + V$ for specific V. There are just three good examples:

- The infinite square well.
- The harmonic oscillator $V = x^2$.
- The Coulomb potential $V = -\frac{1}{\|x\|}$ in $d=3$.

One should keep in mind that $-\Delta \geq 0$, i.e., the kinetic energy is positive. This is a good exercise, in fact.

Exercise 7. Prove the operator inequality $-\Delta \geq 0$. Since $-\Delta = P^2$ and P is self-adjoint, this should be obvious.

4.1 Infinite square well

Formally, we choose $V(x) = \begin{cases} 0 & \text{if } 0 \leq x_j \leq L \ \forall j=1,\dots,d \\ \infty & \text{otherwise.}\end{cases}$

Precisely, we consider the Hamiltonian $H = -\Delta$ on $L^2([0,L]^d)$ with Dirichlet boundary conditions. The particle is then restricted to the box $[0,L]^d$. In contrast to the classical situation, the possible energies form a discrete set.