QUANTUM MECHANICS

1. Motivation

Double-slit experiment: classical prediction is incorrect, particles can be wave-like. See [Sha80, Ch.3]. Each particle is associated with a wave ψ, for which $|\psi(x)|^2$ gives the probability density of finding the particle at x.

2. Axioms of quantum mechanics

The axioms will let us fill out the following chart.

	Classical mechanics	$\longrightarrow$	Quantum mechanics
Particle	$(x(t), p(t))$		$\lvert\psi_t\rangle \in \mathscr{H}$
Momentum	p		$P = -i\hbar\nabla$
Position	x		X mult. op., $X\psi(x) = x\psi(x)$
Hamiltonian	$\mathcal{H} = T + V = \frac{p^2}{2m} + V(x)$		$H = -\frac{\hbar^2}{2m}\Delta + V$
	$\{x, p\} = 1$		$[X, P] = i\hbar$
Time evolution	$\dot{x} = \frac{\partial\mathcal{H}}{\partial x}, \dot{p} = -\frac{\partial\mathcal{H}}{\partial x}$		$i\hbar\frac{\partial}{\partial t}\lvert\psi_t\rangle = H\lvert\psi_t\rangle$

We'll assume that the Hamiltonian $H = T + V$ has no time dependence. Axioms from [Tes14]:

2.1. **Axiom 1.** *The configuration space of a quantum system is a complex separable Hilbert space $\mathscr{H}$. The possible states of the system are represented by elements of $\mathscr{H}$ that have norm one.*

Usually $\mathscr{H} = L^2(\mathbb{R}^d)$. The possible states ψ are called "kets" and often written in bra-ket notation as $|\psi\rangle$, or $|\psi_t\rangle$ if considering time evolution. The norm squared, $|\psi|^2$, gives the probability density for finding the particle in a certain region S, $\int_S |\psi(x)|^2\, dx$.

Some notation involving kets: The inner product is $\langle f|g\rangle = \int \overline{f}g$. Projection onto a state $|\psi\rangle$ is $P = |\psi\rangle\langle\psi|$, i.e. $P|\varphi\rangle = |\psi\rangle\langle\psi|\varphi\rangle$. For an orthonormal basis $(\varphi_j)_j$, then the identity can be written $I = \sum_j |\varphi_j\rangle\langle\varphi_j|$. For kets $|\psi\rangle$ where it makes sense to talk about $\psi(x)$, there is the notation $\langle x|\psi\rangle = \psi(x)$, by viewing $|x\rangle$ as Dirac delta.

2.2. **Axioms 2/3.** (simplified) *Observables correspond to self-adjoint operators. The expectation value of an operator A, in the state $\psi \in \mathfrak{D}(A)$, is*

$$\mathbb{E}_\psi(A) = \langle\psi, A\psi\rangle = \langle A\psi, \psi\rangle \in \mathbb{R}.$$

In physics notation, the inner product is written $\langle\psi|A|\psi\rangle$. Since A is self-adjoint, there is the spectral theorem $A = \int_{\mathbb{R}} \lambda\, dP_\lambda$. When A is unbounded it has to come with a domain $\mathfrak{D}(A) \subset \mathscr{H}$, which will not be discussed here.

The typical observables we are interested in are position, momentum, and total energy. For this talk these will correspond to the operators X, P, and H in the table at the beginning. A

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crucial observation is that X and P as operators do not commute! Defining the commutator $[X, P] := XP - PX$, we compute for ψ nice enough,

$$\langle x|(XP - PX)|\psi\rangle = -i\hbar\,(x \cdot \nabla\psi(x) - \nabla(x\psi(x))) = i\hbar\langle x|\psi\rangle,$$

so that $[X, P] = i\hbar$.

Remark 2.1. Since $XP \neq PX$, it is not immediately clear how to quantize classical expressions involving both x and p, like xp or px. However, one can choose a quantization method such as *Weyl quantization* to handle quantization of general symbols $a = a(x, p)$; see [Zwo12, Ch.4] for the definition.

2.3. **Axiom 4.** *The time evolution is given by a strongly continuous one-parameter unitary group $U(t)$. The generator of this group is the Hamiltonian $H = \frac{P^2}{2m} + V$.*

This axiom governs time evolution according to the Schrödinger equation: If the system starts in the state $|\psi_0\rangle \in \mathfrak{D}(H)$ at $t = 0$, then the Schrödinger equation asserts that

$$i\hbar\frac{\partial}{\partial t}|\psi_t\rangle = H|\psi_t\rangle.$$

The solution is

$$|\psi_t\rangle = e^{-\frac{it}{\hbar}H}|\psi_0\rangle.$$

We call $U(t) = e^{-\frac{it}{\hbar}H}$ the *propagator*; this is the unitary group in Axiom 4 that governs time evolution of the quantum system.

Theorem 2.1. *Let A be self-adjoint and let $U(t) = e^{-itA}$. Then $U(t)$ is a strongly continuous one-parameter unitary group. If $\psi \in \mathfrak{D}(A)$, then $\lim_{t\to 0} \frac{1}{t}(U(t)\psi - \psi) = -iA\psi$.*

Conversely, we have Stone's theorem. It gives a one-to-one correspondence between (one-parameter strongly continuous) unitary groups and self-adjoint operators.

Theorem 2.2 (Stone)**.** *Let $U(t)$ be a weakly continuous one-parameter unitary group. Then its generator A is self-adjoint and $U(t) = e^{-itA}$.*

(Note, weak continuity with the condition $\limsup \|U(t)\psi\| \leq \|U(t_0)\psi\|$ implies strong continuity.) The generator is given by $A\psi = \lim_{t\to 0} \frac{i}{t}(U(t)\psi - \psi)$, $\mathfrak{D}(A) = \{\psi \in \mathscr{H} : \lim_{t\to 0} \frac{1}{t}(U(t)\psi - \psi) \text{ exists}\}$.

To compute $U(t)$, then one just needs to know the spectral data of H which determines $e^{-\frac{it}{\hbar}H}$ by the spectral theorem. Thus we will be interested in solving the so-called *time-independent Schrödinger equation*, $H|\psi\rangle = E|\psi\rangle$, which is just the eigenvalue equation. While many quantum systems have continuous spectrum as well, our main focus will be on eigenvectors.

Remark 2.2. Physicists usually don't like to specify the Hilbert space. The Stone–von Neumann theorem kind of justifies this as long as there is the commutation relation $[X, P] = i\hbar$. (See [Hal13] for details.) Morally, if $[A, B] = i\hbar$ and A, B act irreducibly on $\mathscr{H}$, then A and B are unitarily equivalent to the position and momentum operators X and P on $L^2(\mathbb{R})$. (There is a similar statement for $L^2(\mathbb{R}^n)$.) This isn't exactly correct because of domain issues, in fact we can get counterexamples, but we can fix it by requiring some stronger commutation relations instead.

Theorem 2.3 (Stone–von Neumann)**.** *Let A, B be self-adjoint operators on $\mathscr{H}$ satisfying $[A, B] = i\hbar$. Suppose they also act* irreducibly *on $\mathscr{H}$, i.e. the only closed subspaces of $\mathscr{H}$ invariant under e^{itA} and e^{itB} are $\{0\}$ and $\mathscr{H}$, and that they also satisfy the* exponentiated commutation relations *listed in* [Hal13, Def.14.2/p.284]. *Then there is a unitary map* $U : \mathscr{H} \to L^2(\mathbb{R})$ *such that*

$$Ue^{itA}U^{-1} = e^{itX}$$
$$Ue^{itB}U^{-1} = e^{itP}.$$

If A, B *do not act irreducibly on* $\mathscr{H}$*, we can decompose* $\mathscr{H}$ *as an orthogonal direct sum of closed subspaces* $\{V_l\}$ *such that each* V_l *is invariant under* e^{itA}, e^{itB} *for all* t*, and there exist unitary operators* $U_l : V_l \to L^2(\mathbb{R})$ *such that*

$$U_l e^{itA}U_l^{-1} = e^{itX}$$
$$U_l e^{itB}U_l^{-1} = e^{itP}.$$

3. Examples

3.1. **Particle in a box.** In handwritten notes.

3.2. **Tunneling.** In handwritten notes. Agmon reference is [Agm82].

4. Harmonic oscillator

This mostly follows [Sha80, §7.4-7.5]. The harmonic oscillator Hamiltonian in 1D is

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V, \quad \text{with } V(x) = \frac{1}{2}\omega^2 x^2.$$

Note that $H \geq 0$. We will find all the eigenvalues and eigenvectors of H using the "algebraic method". The idea, due to Dirac, is that $H \sim P^2 + X^2 \sim (X - iP)(X + iP)$, so we can try to "factor" the Hamiltonian. Define

$$a = \left(\frac{m\omega}{2\hbar}\right)^{1/2} X + i\left(\frac{1}{2m\omega\hbar}\right)^{1/2} P$$
$$a^\dagger = \left(\frac{m\omega}{2\hbar}\right)^{1/2} X - i\left(\frac{1}{2m\omega\hbar}\right)^{1/2} P.$$

One can check that $[a, a^\dagger] = 1$, so they don't commute in the "factorization", but still $a^\dagger a = \frac{1}{\hbar\omega}H - \frac{1}{2}$, which leads to the key observation,

$$\boxed{H = \left(a^\dagger a + \frac{1}{2}\right)\hbar\omega}.$$

For convenience, define $\widehat{H} := \frac{H}{\hbar\omega} = a^\dagger a + \frac{1}{2}$. We want to solve for eigenvalues and eigenvalues, $\widehat{H}|\varepsilon\rangle = \varepsilon|\varepsilon\rangle$, where ε is the eigenvalue and $|\varepsilon\rangle$ is the corresponding eigenvector. First we will find the eigenvalues.

4.1. **Eigenvalues.** Why are a and $a^\dagger$ useful? Given an eigenstate of $\widehat{H}$, the operators a and $a^\dagger$ generate other eigenstates. To see this, first it is useful to compute $[a, \widehat{H}] = [a, a^\dagger a + \frac{1}{2}] = [a, a^\dagger a] = a$ and $[a^\dagger, \widehat{H}] = -a^\dagger$. Then given an eigenstate $|\varepsilon\rangle$, consider the vector $a|\varepsilon\rangle$, and compute

$$\widehat{H}a|\varepsilon\rangle = (a\widehat{H} - [a, \widehat{H}])|\varepsilon\rangle = (a\widehat{H} - a)|\varepsilon\rangle = (\varepsilon - 1)a|\varepsilon\rangle.$$

Thus $a|\varepsilon\rangle$ is a (possibly unnormalized) eigenvector with eigenvalue $\varepsilon - 1$. Letting $|\varepsilon - 1\rangle$ be a normalized state, then we have $a|\varepsilon\rangle = C_\varepsilon|\varepsilon - 1\rangle$ for a constant C_ε to be determined later. Similarly,

$$\widehat{H}a^\dagger|\varepsilon\rangle = (a^\dagger\widehat{H} - [a^\dagger, \widehat{H}])|\varepsilon\rangle = (a^\dagger\widehat{H} + a^\dagger)|\varepsilon\rangle = (\varepsilon + 1)a^\dagger|\varepsilon\rangle,$$

so that $a^\dagger|\varepsilon\rangle$ is an eigenvector with eigenvalue $\varepsilon+1$. Thus a is called the lowering operator or destruction operator, and $a^\dagger$ is called the raising operator or creation operator. (They create or destroy energy $\hbar\omega$.)

Now if ε is an eigenvalue of $\widehat{H}$, then so are $\varepsilon+1, \varepsilon+2, \dots$ and $\varepsilon-1, \varepsilon-2, \dots$. But we know that $H \geq 0$, so the bottom ladder chain cannot continue to $-\infty$; there must be some state $|\varepsilon_0\rangle$ where $a|\varepsilon_0\rangle = 0$, the zero vector. Again using the ladder operators a and $a^\dagger$, we can solve for this ε_0:

$$a|\varepsilon_0\rangle = 0 \implies a^\dagger a|\varepsilon_0\rangle = 0 \implies (\widehat{H} - 1/2)|\varepsilon_0\rangle \implies \widehat{H}|\varepsilon_0\rangle = \frac{1}{2}|\varepsilon_0\rangle,$$

so $\varepsilon_0 = \frac{1}{2}$ is the lowest energy, or ground state. Thus we know that H has at least the eigenvalues $E_n = (n+1/2)\hbar\omega$ for $n \in \mathbb{N}_0$. In fact by finding a full eigenbasis for these eigenvalues, we will show that this is the entire spectrum of H.

4.2. **Eigenvectors.** It will be convenient to index the states by n, so that $\widehat{H}|n\rangle = (n+1/2)|n\rangle$, and $|n\rangle$ is the result of starting in a ground state $|0\rangle$ and applying the raising operator, $a^\dagger$, n times and normalizing. Now we will need to compute these normalizing constants. Recall $a|n\rangle = C_n|n-1\rangle$. Then

$$|C_n| = \|a|n\rangle\| = \langle n|a^\dagger a|n\rangle^{1/2} = \langle n|\widehat{H} - 1/2|n\rangle^{1/2} = \langle n|n|n\rangle^{1/2} = n^{1/2}.$$

By convention, we choose $C_n = n^{1/2}$ real. The computation for $a^\dagger$ is similar, and results in

$$\begin{aligned} a|n\rangle &= n^{1/2}|n-1\rangle \\ a^\dagger|n\rangle &= (n+1/2)^{1/2}|n+1\rangle \\ a^\dagger a|n\rangle &= a^\dagger n^{1/2}|n-1\rangle = n|n\rangle. \end{aligned}$$

Because of the last equation, $N = a^\dagger a$ is called the *number operator* since it returns the state number n.

Remark 4.1. Assuming that these vectors indexed by n form a basis, this makes it easy to compute matrix elements of $X = \left(\frac{\hbar}{2m\omega}\right)^{1/2}(a+a^\dagger)$ and $P = i\left(\frac{m\omega\hbar}{2}\right)^{1/2}(a^\dagger - a)$ in the eigenbasis, using for example that $\langle n'|a|n\rangle = n^{1/2}\delta_{n',n-1}$.

Now we compute the eigenvectors in the position basis and show they form a complete (Schauder) basis. These will be denoted $\psi_n(x) = \langle x|n\rangle$.

First, we can find the ground state $|0\rangle$. To simplify the constants, let $y := \left(\frac{m\omega}{\hbar}\right)^{1/2} x$. Then $a = \frac{1}{\sqrt{2}}(y + \frac{\partial}{\partial y})$ and $a^\dagger = \frac{1}{\sqrt{2}}(y - \frac{\partial}{\partial y})$ (since $\frac{\partial}{\partial y}$ is anti-hermitian). Letting $\psi_0(x) = \langle x|0\rangle$, the equation $a|0\rangle = 0$ becomes,

$$\begin{aligned} \left(y + \frac{\partial}{\partial y}\right)\psi_0(y) &= 0 \\ \frac{\partial}{\partial y}\psi_0(y) &= y\psi_0(y) \\ \implies \psi_0(y) &= Ce^{-y^2/2} = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega x^2}{2\hbar}}. \end{aligned}$$

Since

$$|n\rangle = \frac{(a^\dagger)^n}{(n!)^{1/2}}|0\rangle,$$

then

$$\psi_n(x) = \langle x|n\rangle = \frac{1}{(n!)^{1/2}}\left[\frac{1}{\sqrt{2}}\left(y - \frac{\partial}{\partial y}\right)\right]^n \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-y^2/2}. \tag{4.1}$$

The Hermite polynomials are defined by

$$H_n(y) := e^{y^2/2}\left(y - \frac{\partial}{\partial y}\right)^n e^{-y^2/2},$$

and the first few Hermite polynomials are

$$\begin{aligned} H_0(y) &= 1 \\ H_1(y) &= 2y \\ H_2(y) &= -2(1-2y^2) \\ &\vdots \end{aligned}$$

They satisfy the recurrence relation $H_{n+1}(y) = 2yH_n(y) - 2nH_{n-1}(y)$. The eigenfunctions ψ_n in (4.1) are then Hermite polynomials times $e^{-y^2/2}$, which span $D := \operatorname{span}(x^k e^{-x^2/2},\, k \in \mathbb{N}_0)$, with just finite linear combinations. To show the orthonormal system of eigenfunctions is a basis for $L^2(\mathbb{R})$, we show D is dense, which also shows that if $\langle\varphi|\psi_n\rangle = 0$ for all $n \in \mathbb{N}_0$, then $\varphi \equiv 0$. Let $\varphi \in D^\perp$, so $\langle\varphi|\psi\rangle = 0$ for all $\psi \in D$. Then

$$\int \overline{\varphi}(x) x^k e^{-x^2/2}\, dx = 0, \quad \forall k \in \mathbb{N}_0.$$

The Fourier transform of $\overline{\varphi}(x)e^{-x^2/2}$ is

$$F(\xi) = \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} \overline{\varphi}(x)e^{-x^2/2}\sum_{j=1}^{\infty}\frac{(-i\xi x)^j}{j!}\, dx = 0,$$

by dominated convergence, so $\overline{\varphi}(x)e^{-x^2/2} \equiv 0$ and $\varphi \equiv 0$. Thus the eigenfunctions in (4.1) form an orthonormal (Schauder) basis for $L^2(\mathbb{R})$.

4.3. **Propagator.** Now that we know an eigenbasis for H, the propagator is

$$U(t) = e^{-\frac{it}{\hbar}H} = \sum_{n=0}^{\infty} e^{-i(n+1/2)\omega t}|\psi_n\rangle\langle\psi_n|.$$

This sum is difficult to evaluate, but we will later obtain an easy formula from the path integral method. One can also compute $e^{-\frac{it}{\hbar}H}$ by computing the heat kernel $\langle x|e^{-tH}|y\rangle$ using the Feynmann–Kac formula, then plugging in $t \mapsto it$.

References

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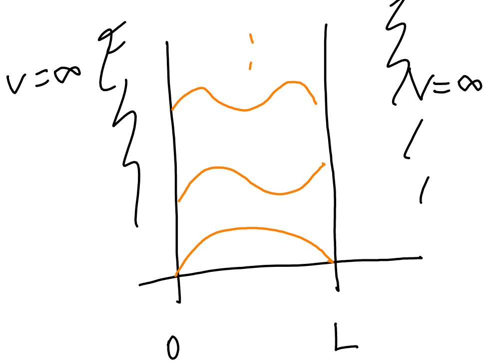
Examples

1.) Particle in a box

2.) Tunneling

3.) Harmonic oscillator

1.) Particle in a box



$$H = -\frac{d^2}{dx^2}, \qquad \psi(0) = \psi(L) = 0$$

$$H|\psi\rangle = k^2|\psi\rangle \qquad (H \geq 0)$$

$$-\frac{d^2}{dx^2}\psi(x) = k^2\psi(x)$$

$$\Rightarrow \psi(x) = C_1 e^{ikx} + C_2 e^{-ikx} \qquad k > 0$$

$$\psi(0) = C_1 + C_2 = 0$$

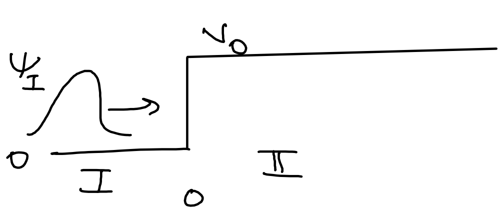
$$\psi(L) = C_1 e^{ikL} - C_1 e^{-ikL} = 0$$

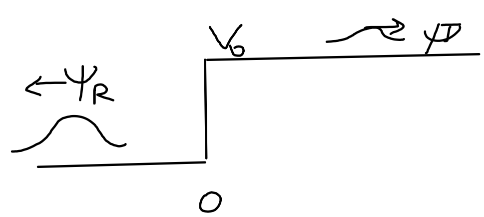
$$\Leftrightarrow \sin(kL) = 0 \quad \Leftrightarrow \quad k \in \frac{\pi}{L}\mathbb{Z}$$

$$\Rightarrow \psi_k(x) = \sqrt{\frac{2}{L}}\cdot\sin(kx), \quad k \in \frac{\pi}{L}\mathbb{Z}_+$$

$$E = k^2$$

2.) Tunneling





Solve:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi_I(x) = E\Psi_I(x)$$

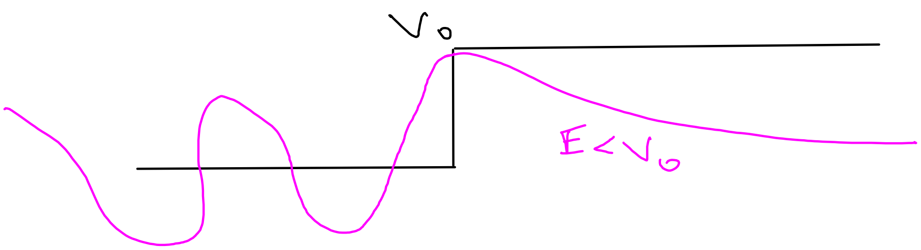
B.C. continuity + cts deriv

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\Psi_{II}(x) + V_0\Psi_{II}(x) = E\Psi_{II}(x)$$

$$\psi_{I}(x) = Ae^{ikx} + Be^{-ikx} \qquad k = \frac{\sqrt{2mE}}{\hbar}$$

If $E < V_0$ classically forbidden

$$\psi_{II}(x) = \cancel{Ce^{\beta x}} + De^{-\beta x}, \qquad \beta = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$



More generally:
PDE
Agmon estimates
for $-\Delta + V$
exp. decay outside
potential wells

$\{V(x) \leq E\}$

Tunneling