Quantum Mechanics I

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1 Classical Mechanics

In order to later compare quantum mechanics, let us first introduce some classical mechanics.

In classical mechanics, we study classical objects/particles which has a mass $m \in \mathbb{R}$ and a state. In particular, the state of the particle is represented by its position, commonly $r \in \mathbb{R}^3$, and its velocity $v = \dot{r} \in \mathbb{R}^3$. More conveniently, we can also represent the velocity in terms of its momentum $p = mv$.

We recall Newton's second law which describes how the state of a particle changes in time in the presence of external forces. That is,

$$\dot{p} = F(r),$$

where F is the external force depending on r.

As the state of a particle is represented by its position and momentum, visually the state of a particle can be represented by a phase-space with a trajectory corresponding to $(r(t), p(t))$.

An another formulation of classical mechanics is Hamilton's formulation. While Hamilton's formulation is very powerful, it does not apply to every classical system. In particular, Hamilton's formulation requires the system to be conservative.

Definition 1.1 (Conservative)**.** A classical system is said to be conservative if

$$F(r) = -\nabla V(r),$$

where V is the potential given the position.

Definition 1.2 (Hamiltonian Function)**.** The Hamiltonian function H is defined as

$$H(p, q) = \frac{p^2}{2m} + V(q),$$

where $p^2/2m$ is the kinetic energy and V the potential.

Thus, with the definition of conservative in mind, we see that for a one dimensional system with position given by $q \in \mathbb{R}$, we have

$$\dot{p} = F(q) = -\frac{\partial V}{\partial q} \text{ and } \dot{q} = \frac{p}{m}.$$

Writing in terms of the Hamiltonian function, we obtain,

$$\dot{p} = -\frac{\partial H}{\partial q} \text{ and } \dot{q} = \frac{\partial H}{\partial p}.$$

These two equations are known as Hamilton's canonical equations and describe the motion of a particle in a conservative system. The theory itself is more general in which we simply require p, q to be canonically conjugate variables.

Example 1.1 (Free Particle)**.** Consider a free particle with $V(q) = 0$ (thus, $H = p^2/2m$), we have the canonical equations $\dot{p} = 0$ and $\dot{q} = p/m$, and thus, $p(t) = p(0)$ and $q(t) = q(0) + \frac{p}{m}t$.

Example 1.2 (Harmonic Oscillator)**.** A harmonic oscillator is described by $V(q) \propto q^2$. By similar calculation we find $\ddot{q} = -\frac{2k}{m}q$ for some k such that $V = kq^2$.

As for a particle in classical mechanics, the state is given by its position and momentum, any measurable quantity A is given as a function $A(p,q)$ such that

$$\frac{\mathrm{d}A}{\mathrm{d}t} = \frac{\partial A}{\partial p}\dot{p} + \frac{\partial A}{\partial q}\dot{q} + \frac{\partial A}{\partial t}.$$

Substituting the Hamiltonian equations, we have

$$\frac{\mathrm{d}A}{\mathrm{d}t} = -\frac{\partial A}{\partial p}\frac{\partial H}{\partial q} + \frac{\partial A}{\partial q}\frac{\partial H}{\partial p} + \frac{\partial A}{\partial t} = \frac{\partial A}{\partial q}\frac{\partial H}{\partial p} - \frac{\partial A}{\partial p}\frac{\partial H}{\partial q} + \frac{\partial A}{\partial t}.$$

As the first term of this equation is very common, we denote it as $\{H, A\}$ such that

$$\frac{\mathrm{d}A}{\mathrm{d}t} = \{H, A\} + \frac{\partial A}{\partial t}.$$

Similarly, for general variables F, G,

$$\{F, G\} := \sum_{n=1}^{N} \frac{\partial F}{\partial p_n}\frac{\partial G}{\partial q_n} - \frac{\partial F}{\partial q_n}\frac{\partial G}{\partial q_n},$$

and is known as the Poisson bracket of F and G.

Definition 1.3 (Poisson Bracket)**.** A Poisson bracket is simply any bracket of functions satisfying

- $\{A, A\} = 0$;
- $\{c_1 A + c_2 B, C\} = c_1\{A, C\} + c_2\{B, C\}$;
- $\{A, B\} = -\{B, A\}$.
- $\{c, A\} = 0$ for any constant c;
- $\{AB, C\} = A\{B, C\} + \{A, C\}B$ (Leibniz rule);
- $\{A, \{B, C\}\} + \{B, \{C, A\}\} + \{C, \{A, B\}\} = 0$ (Jacobi identity).

As an exercise, one may check that the Poisson bracket defined above is indeed a Poisson bracket.

Proposition 1.1. $\{p, q\} = 1$ and in higher dimensions. $\{p_i, q_j\} = \delta_{ij}$.

Definition 1.4 (Canonical Conjugate Variables)**.** $P(p,q), Q(p,q)$ are called canonical conjugate variables if $\{P, Q\} = 1$. Similarly, for higher dimensions, P, Q are canonical conjugates if $\{P_i, Q_j\} = \delta_{ij}$.

Proposition 1.2. For any pair of canonical conjugate variables P, Q, we have

$$\dot{P}_j = -\frac{\partial H}{\partial Q_j} = \{H, P_j\} \text{ and } \dot{Q}_j = \frac{\partial H}{\partial P_j} = \{H, Q_j\}.$$

2 Schödinger Dynamics

The Scrhödinger equations is a function of position and time which is written in its compact form as

$$i\hbar\dot{\psi} = \hat{H}\psi$$

where $\hat{H}$ is known as the Hamiltonian and $\hbar = h/2\pi$ where h is Plank's constant.

Similar to the Hamiltonian in classical mechanics, the Hamiltonian is an linear operator that often encodes energy and in that case, it is written as

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(r),$$

where ∇^2 is the Laplacian operator. Furthermore, the expectation of the Hamiltonian, defined by

$$\langle\hat{H}\rangle := \frac{1}{\int_{\mathbb{R}^n} |\psi|^2 \mathrm{d}x^n} \int_{\mathbb{R}^n} \psi^* \hat{H}\psi \mathrm{d}x^n$$

provides the total energy of the system. As $\hat{H}$ is a linear operator, it has eigenfunctions where ϕ_E is said to be an eigenfunction if $\hat{H}\phi_E = E\phi_E$ and this equation is known as the time-independent Schrödinger equation. It is possible to show that this eigenfunctions are orthogonal with respect to the L^2 inner product and form an eigenbasis of all possible states of a system.

As the Schrödinger equation is a linear differential equation, the solution space of the equation is a linear space. In particular, if ψ_i are solutions to the Schrödinger equations, so is $c_1\psi_1 + c_2\psi_2$ for c_1, c_2 constants.

The function ψ is known as the wave function and it is interpreted as the probability of finding the particle it describes at a given time in a certain region. As ψ is a complex functions, it values is known as a probability amplitude by while $|\psi|^2$ is the probability distribution function. Thus, the probability of finding a particle is the interval $[a, b]$ is

$$\int_a^b |\psi(x,t)|^2 \mathrm{d}x,$$

if ψ is normalized, i.e. $\int_{-\infty}^{\infty} |\psi(x,t)|\mathrm{d}x = 1$ for all t. In particular, we note that this interpretation is meaningful only if ψ is square integrable, i.e. $\psi \in L^2$.

Let us consider the following 1-dimensional example. Let $\hat{H}$ be the Hamiltonian as described above, then we have the Schödinger equation

$$i\hbar\dot{\psi}(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + V(x)\psi(x,t).$$

Then, defining $N(t) := \int_{-\infty}^{\infty} |\psi(x,t)|^2 \mathrm{d}x$, we have

$$\begin{aligned}\frac{\mathrm{d}N}{\mathrm{d}t} &= \frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{\infty} \psi^*(x,t)\psi(x,t)\mathrm{d}x \\ &= \int_{-\infty}^{\infty} \dot{\psi}^*\psi + \psi^*\dot{\psi}\mathrm{d}x\end{aligned}$$

substituting $\dot{\psi}$ and $\dot{\psi^*}$ using the Schrödinger equation, we have

$$\begin{aligned}\frac{\mathrm{d}N}{\mathrm{d}t} &= \frac{i}{\hbar}\int_{-\infty}^{\infty}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi^* + V\psi^*\right)\psi - \psi^*\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + V\psi\right)\mathrm{d}x \\ &= \frac{i\hbar}{2m}\int_{-\infty}^{\infty}\psi\frac{\partial^2}{\partial x^2}\psi^* - \psi^*\frac{\partial^2}{\partial x^2}\psi\mathrm{d}x \\ &= \frac{i\hbar}{2m}\int_{-\infty}^{\infty}\frac{\partial}{\partial x}\left(\psi\frac{\partial}{\partial x}\psi^* - \psi^*\frac{\partial}{\partial x}\psi\right)\mathrm{d}x \\ &= 0\end{aligned}$$

where the last equality follows by the fundamental theorem of calculus and the fact that $\psi \in L^2$. Thus, N is conserved over time and we may normalize ψ by simply divide by N.

Definition 2.1 (Probability Flux)**.** The probability flux of a wave function ψ is defined as

$$j(x,t) := \frac{i\hbar}{2m}\left(\psi^*\frac{\partial}{\partial x}\psi - \psi\frac{\partial}{\partial x}\psi^*\right).$$

In particular, we see that $\frac{\partial|\psi|^2}{\partial t} = -\frac{\partial j}{\partial x}$, and so, we have the continuity equation

$$\frac{\partial|\psi|^2}{\partial t} + \frac{\partial j}{\partial x} = 0.$$

Unlike the total probability N, the probability in a certain region does fluctuate over time and we see that, if $P_{[a,b]}(t)$ is the probability that a particle is in the region $[a,b]$ at time t, then

$$\frac{\mathrm{d}P_{[a,b]}}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\int_a^b |\psi|^2\mathrm{d}x = -\int_a^b \frac{\partial j}{\partial x}\mathrm{d}x = j(a,t) - j(b,t).$$

Similarly, for higher dimensions, we define the probability flux of ψ as

$$j(r,t) = \frac{\hbar}{2mi}(\psi^*\nabla\psi - \psi\nabla\psi^*),$$

and we have the continuity equation

$$\frac{\partial|\psi|^2}{\partial t} + \nabla\cdot j = 0.$$

Then, if P_V is the probability of finding a particle in the region V, we have

$$\frac{\mathrm{d}P_V}{\mathrm{d}t} = -\int_V \nabla\cdot j\mathrm{d}V = -\int_S j\cdot\mathrm{d}S$$

by the divergence theorem. Thus, the probability change is the total flux through the boundary of the volume.

2.1 Stationary Solution

Let us consider a special family of solutions. Consider the Schrödinger equation

$$i\hbar\dot{\psi} = \hat{H}\psi,$$

where ψ is expressible in the form $\psi(r,t) = \phi(r)\chi(t)$. Then, we have

$$i\hbar\dot{\chi}(t)\phi(r) = i\hbar\dot{\psi} = \hat{H}\phi(r)\chi(t) = \chi(t)\hat{H}\phi(r),$$

and so,

$$i\hbar\frac{\dot{\chi}(t)}{\chi(t)} = \frac{\hat{H}\phi(r)}{\phi(r)}.$$

By observing that the right hand side and the left hand sides of the equation depend on different variables, we conclude that both values must be constants and we denote this constant by E such that

$$\dot{\chi}(t) = -\frac{i}{\hbar}E\chi(t), \text{ and } \hat{H}\phi(r) = E\phi(r).$$

Thus, solving the first differential equation, we have

$$\chi(t) = e^{-iEt/\hbar}\chi(0),$$

while the second is the time-independent Schrödinger equation. The time-independent Schrödinger equation is not always easy to solve though it is solvable analytically in special cases. In particular, for Hamiltonians in of form $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$ where the potient V tends to ∞ as $x \to \infty$, normalizable solutions to the time-independent Schrödinger equation only exist for special discrete values of E.

In this case, the wave function is simply

$$\psi(r,t) = \chi_0 e^{-iEt/\hbar}\phi_E(r),$$

and if $\psi(r,0) = \phi(r)$ the probability distribution of the particle is $|\psi(r,t)|^2 = |\phi_E(r)|^2$ which is independent of time, and thus we call solutions of this form stationary states. Note that the superposition of stationary states is not necessarily stationary (exercise).

3 Principles

3.1 Mathematics Review

Let us recall some definitions which is required for quantum mechanics.

Definition 3.1 (Inner Product Space)**.** A inner product space is a vector space V equipped with a map $\langle \cdot, \cdot \rangle : V \times V \to \mathbb{C}$ such that for all $u, v, w \in V, \lambda, \mu \in \mathbb{C}$,

- $\langle u, v \rangle = \langle v, u \rangle^*$;
- $\langle u, u \rangle \geq 0$ with equality if and only if $u = 0$;
- $\langle u, \lambda v + \mu w \rangle = \lambda \langle u, v \rangle + \mu \langle u, w \rangle$.

Recall that inner product induces a norm by defining $\| \cdot \| : V \to \mathbb{R} : v \mapsto \sqrt{\langle v, v \rangle}$.

Definition 3.2 (Complete)**.** A topological space is complete if every Cauchy sequence converge in that space.

Definition 3.3 (Separable)**.** A topological space is separable if there exists a countable dense subset.

Definition 3.4 (Hilbert Space)**.** A Hilbert space is a inner product space such that the induced topology is complete and is separable[1].

In finite dimensional spaces, an inner product space is automatically complete and separable. In particular, a finite dimensional inner product space over $\mathbb{R}$ or $\mathbb{C}$ is complete and separable since $\mathbb{R}$ and $\mathbb{C}$ are complete and separable.

Definition 3.5 (Linear Operator)**.** A linear operator is simply a function belonging to $\mathrm{End}(V)$.

As linear operators are simply linear maps, definitions such as eigenvalues and eigenvectors are defined analogously.

Definition 3.6 (Adjoint Operator)**.** Given a linear operator $A : V \to V$, the adjoint of A is a linear operator $A^\dagger$ such that

$$\langle Au, v \rangle = \langle u, A^\dagger v \rangle$$

for all $u, v \in V$.

Definition 3.7 (Self-Adjoint Operator)**.** A linear operator A is self-adjoint if $A = A^\dagger$ and an operator satisfying this property is refereed to as a Hermitian operator.

Recalling the spectral theorem from second year, we have that the eigenvalues of a self-adjoint operator are real and furthermore, its eigenvectors form a basis and are orthogonal. One may also show that for A is Hermitian if and only if the expectation values $\langle v, Av \rangle$ are real for all $v \in V$.

Definition 3.8 (Dual Space)**.** The dual space of a vector space V is the vector space of linear functionals of V.

Recall that the dual space of a vector space is (non-canonically) isomorphic to that space, and this is summarized by the Riesz representation theorem.

[1] We note that the condition for separability is normally omitted for in mathematical contexts.

Theorem 1 (Riesz Representation Theorem)**.** Every Hilbert space $\mathcal{H}$ is (anti-)isomorphic to its dual space. In particular, there exists a bijective map between the linear functionals $F \in \mathcal{H}^*$ and vectors $f \in \mathcal{H}$ such that $F(\phi) = \langle f, \phi \rangle$ for all $\phi \in \mathcal{H}$.

Proof. See last year for the finite dimensional case while the general case can be found in the functional analysis course. □

3.2 Dirac Notation

Given a vector ϕ in the Hilbert space $\mathcal{H}$, we denote ϕ by $|\phi\rangle$ and we call it a "ket"-vector. On the other hand, given $F = \phi \mapsto \langle f, \phi \rangle \in \mathcal{H}^*$ we denote F by $\langle f|$ and we call it a "bra"-vector. With this, we denote

$$F(\phi) = \langle f, \phi \rangle = \langle f | \phi \rangle .$$

If A is a linear operator, it makes sense to denote $A|\phi\rangle$ by the ket-vector $|A\phi\rangle$. On the other hand, if $|\chi\rangle := A|\phi\rangle$, we see that, for all $\psi \in \mathcal{H}$,

$$\langle \chi | \psi \rangle = \langle A\phi, \psi \rangle = \langle \phi, A^\dagger \psi \rangle = \langle \phi | A^\dagger | \psi \rangle .$$

Hence, we denote the linear operator $\langle \chi| = \langle A\phi, \cdot \rangle$ by the notation $\langle \phi| A^\dagger$. Thus, the notation $\langle \phi| A |\psi\rangle$ might denotes two equal equations, i.e. $\langle A^\dagger \phi, \psi \rangle = \langle \phi| A |\psi\rangle = \langle \phi, A\psi \rangle$.

Given an expression in Dirac notation, there are a set of easy rules for finding the adjoint of that expression (easy check by unfolding definitions). In particular, to find the adjoint, one needs to replace

- $c \leftrightarrow c^*$ for scalars c;
- $\langle \phi| \leftrightarrow |\phi\rangle$ for vectors ϕ;
- $A \leftrightarrow A^\dagger$ for linear operators A;
- reverse the order of factors.

By definition, we have $\langle \phi | \psi \rangle = \langle \phi, \psi \rangle$ is the inner product of ϕ and ψ. On the other hand, one can define the outer product by $|\phi\rangle \langle \psi|$ which is a linear operator such that $|\chi\rangle \mapsto |\phi\rangle \langle \psi | \chi \rangle = \langle \psi | \chi \rangle |\phi\rangle$. In the case that $\phi = \psi$, we see that the operator $|\phi\rangle \langle \phi|$ is the projection operator on to the vector ϕ.

Now, if $\{|\phi_n\rangle\}$ is countable basis of a Hilbert space $\mathcal{H}$, then for all $|\chi\rangle \in \mathcal{H}$, we have

$$|\chi\rangle = \sum_n \chi_n |\phi_n\rangle .$$

Then, if $\{|\phi_n\rangle\}$ is orthonormal, we have

$$|\chi\rangle = \sum_n \langle \phi_n | \chi \rangle |\phi_n\rangle = \sum_n |\phi_n\rangle \langle \phi_n | \chi \rangle = (\sum_n |\phi_n\rangle \langle \phi_n|) |\chi\rangle .$$

Thus, the operator $\sum_n |\phi_n\rangle \langle \phi_n|$ is the identity operator.

3.3 Principles of Quantum Mechanics

Quantum mechanics is built upon principles on which all results follow. They are like the axioms in mathematics from which all states can eventually reduce down to them.

The first principle states that, the *state* of a quantum system is described by a non-zero vector in a Hilbert space.

We have already seen a application of this principle in Schrödinger dynamics where the Hilbert space is L^2 and the state is described by the wave function $\psi \in L^2$.

Definition 3.9 (State Space)**.** The state space is a projective Hilbert space, i.e. a Hilbert space $\mathcal{H} \setminus \{0\}$ quotiented by the equivalence relation $\sim$ where $x \sim y \iff$ there exists some $c \in \mathbb{C}$ such that $x = cy$.

The second principle states that, a *measurable quantity* is described by a Hermitian operator acting on the Hilbert space. Both the measurable quantity and the operator representing it are refereed to as observables.

Similar to Hamiltonian mechanics, the operators corresponding to position and momentum satisfy some notion of canonical conjugacy. In particular, we have the

$$[p, q] = i\hbar \mathrm{Id},$$

where p is the position operator and q the momentum, and $[\cdot, \cdot]$ is the commutator defined as $[A, B] = AB - BA$. In Schrödinger's formulation, we have the position operator is defined as

$$q : L^2 \to L^2 : \psi(x) \mapsto x\psi(x).$$

With this, the momentum operator is fixed (modulo some addition of operators commuting with q), and we have

$$p : L^2 \to L^2 : \psi \mapsto -i\hbar \frac{\partial \psi}{\partial x}.$$

Definition 3.10 (Projection Operator)**.** A linear operator P is a projection operator if $P^2 = P$.

The third principle (often known as the Born rule) states that, the possible outcomes of a measurement of an observable A are given by the eigenvalues of the corresponding operator A. If the system is described by the state $|\psi\rangle$ immediately before the measurement, then the probability of measuring the value a_j in an A-measurement is given by

$$p(a_j) = \langle \psi | \hat{P}_j | \psi \rangle ,$$

where $\hat{P}_j$ is the projection operator onto a_j-eigenspace.

In the case that the observable have non-degenerate (i.e. the eigenspaces have dimension 1), discrete eigenvalues a_j so that $A|\phi_j\rangle = a_j |\phi_j\rangle$ where $|\phi_j\rangle$ are normalized, we have,

$$p(a_j) = \langle \psi | \hat{P}_j | \psi \rangle = \langle \psi | \phi_j \rangle \langle \phi_j | \psi \rangle = | \langle \phi_j | \psi \rangle |^2.$$

So, by noticing $\langle \phi_j | \psi \rangle$ is the coefficients of ψ in the basis of $\{\phi_j\}$, we have, if $\psi = \sum_n \psi_n |\phi_n\rangle$, then $p(a_j) = |\psi_j|^2$.

For continuous spectra, the situation is similar, in which we obtain

$$|\psi\rangle = \int \mathrm{d}\alpha \psi(\alpha) \, |\phi(\alpha)\rangle$$

and the probability of measuring a value in the interval I is given by

$$p(\alpha \in I) = \int_I |\psi(\alpha)|^2 \mathrm{d}\alpha.$$

Definition 3.11 (Expectation Value)**.** Given an observable A with eigenvalues a_j in the state $|\psi\rangle$, its expectation value is simply

$$\langle A \rangle := \sum_j a_j p(a_j) = \frac{\langle \psi | \, A \, | \psi \rangle}{\langle \psi | \psi \rangle}.$$

The two equations given in the definition are indeed equal since, $p(a_j) = \frac{\langle \psi | \phi_j \rangle \langle \phi_j | \psi \rangle}{\langle \psi | \psi \rangle}$, and so,

$$\langle A \rangle = \sum_j \frac{a_j \langle \psi | \phi_j \rangle \langle \phi_j | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\langle \psi | \left(\sum_j a_j |\phi_j\rangle \langle \phi_j| \right) | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\langle \psi | \, A \, | \psi \rangle}{\langle \psi | \psi \rangle}$$

The fourth principle (known as the state collapse postulate) states that, if $|\psi\rangle$ describes a quantum system on which a measurement of an observable A is performed, then if the measurement yield a_j, the state of system directly after the measurement is given by

$$\frac{\hat{P}_j \, |\psi\rangle}{\sqrt{\langle \psi | \, \hat{P}_j \, | \psi \rangle}},$$

where $\hat{P}_j$ is the projection operator onto the a_j-eigenspace.

Lastly, the fifth principle states that, the time-evolution of a quantum state $|\psi(t)\rangle$ is governed by the Schrödinger equation

$$i\hbar \left| \dot{\psi} \right\rangle = \hat{H} \, |\psi\rangle \, ,$$

where $\hat{H}$ is the operator corresponding to the total energy of the system.

3.4 Commutators and Uncertainty

Given an observable A, the outcome of measurement of A has a certain spread which is characterised by its variance

$$(\Delta A)^2 := \langle (A - \langle A \rangle)^2 \rangle = \langle A^2 \rangle - \langle A \rangle^2.$$

In quantum mechanics we refer to the standard deviation ΔA as the uncertainty of A.

Proposition 3.1. Given two Hermitian operators A, B with $[A, B] \neq 0$, we have

$$\Delta A \Delta B \geq \frac{1}{2} |\langle C \rangle|,$$

where $C := i[A, B]$ (in particular, C is Hermitian).

Proof. We may assume $\langle A\rangle = \langle B\rangle = 0$ without loss of generality. Let $|\chi\rangle := (A - i\lambda B)\,|\phi\rangle$ for some $\lambda \in \mathbb{R}$ and $|\phi\rangle$ a normalized state, we have

$$\begin{aligned}\langle\chi|\chi\rangle &= \langle\phi|\,(A + i\lambda B)(A - i\lambda B)\,|\phi\rangle = \langle (A + i\lambda B)(A - i\lambda B)\rangle \\ &= \langle A^2 + \lambda B + i\lambda(BA - AB) = \langle A^2\rangle + \lambda^2\langle B^2\rangle - \lambda\langle C\rangle.\end{aligned}$$

On the other hand, $\langle\chi|\chi\rangle \geq 0$, and so

$$\langle A^2\rangle + \lambda^2\langle B^2\rangle - \lambda\langle C\rangle \geq 0,$$

for all values $\lambda \in \mathbb{R}$. Taking the derivative of $\langle\chi|\chi\rangle$, we find $\langle\chi|\chi\rangle$ is an extreme at $\lambda = \langle C\rangle/(2\langle B^2\rangle)$, and this is a global minimum as $\langle\chi|\chi\rangle$, is a monic quadratic polynomial. Thus,

$$\langle\chi|\chi\rangle \geq \langle A^2\rangle + \frac{\langle C\rangle^2}{4\langle B^2\rangle^2}\langle B^2\rangle - \frac{\langle C\rangle^2}{2\langle B^2\rangle} = \langle A^2\rangle - \frac{\langle C\rangle^2}{4\langle B^2\rangle} \geq 0,$$

implying $\langle A^2\rangle\langle B^2\rangle \geq \langle C\rangle^2/4$, and hence, as $\Delta A^2 = \langle A^2\rangle - \langle A\rangle^2 = \langle A^2\rangle$ and similarly, $\Delta B^2 = \langle B^2\rangle$, we have

$$(\Delta A)(\Delta B) \geq \frac{|\langle C\rangle|}{2}.$$

□

Proposition 3.2. If A, B are operators such that $[A, B] = 0$, then they possess a set of common eigenvectors.

Definition 3.12 (Complete Set of Commuting Observables)**.** Given a Hibert space $\mathcal{H}$, a set of Hermitian operators $(A_i)_{i\in\mathcal{I}}$ sharing an eigenbasis on $\mathcal{H}$ is called a complete set of commuting observables if their eigenvalues uniquely defines each basis vector up to a phase.

Definition 3.13 (Parity Operator)**.** A Hermitian operator S on L^2 is a parity operator if $S\phi(x) = \phi(-x)$.

We see that if ϕ is an eigenfunction of the parity operator S, then $S\phi(x) = \phi(-x) = s\phi(x)$. Furthermore, if $S^2 = 1$, we have $\phi(x) = S\phi(-x) = S^2\phi(x) = s^2\phi(x)$ implying $s = \pm 1$. It is not difficult to show that a Hamiltonian of the form

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V$$

commutes with S if $V(x) = V(-x)$.

4 Specific Systems

We have so far looked at the formulation of quantum mechanics in a very abstract way. To actually find a solution with these formulations however, is very hard. In general, most solutions will require numerical approximation, but there are some special cases where we can find solutions analytically.

4.1 Properties of Eigenfunctions

Consider a quantum particle in a 1-dimension in an external potential. This system is described by the Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\phi_E(x) = E\phi(X).$$

There are in general two types of solutions to this equation. In particular, if $\phi_E(x \to \pm\infty) \to$ then the state is a bound state and they have discrete energies. Alternatively, the continuum states which has potiential that does not tend to 0 as $x \to \pm\infty$. An example we have already seen is the eigenfunctions for the momentum operator $e^{\pm ikx}$. These solutions are associated with a continuum of energies.

If $V(x \to \pm) \to \infty$, then the only solution are bound states.

Proposition 4.1. The eigenfunctions $\phi_E(x)$ of a 1-dimensional system can always be chosen to be real.

Proof. If $\phi_E(x)$ is a solution to the Schrödinger equation, then so is $\phi_E^*(x)$ and thus, $\phi_E + \phi_E^*$ is a solution which is real. □

Proposition 4.2. There are no bound states with energy less than the minimum of $V(x)$.

Proof. Rewritting the Schrödinger equation, we have

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

So, if $E < V_{\min} \leq V$, then $\phi_E''(x) > 0$ for all x. But then ϕ_E is not normalizable and thus, cannot be a state. □

Proposition 4.3. The expectation of the energy is bounded below by the lowest energy eigenvalue.

Proof. Proven later. □

Proposition 4.4. The bound state eigenvalues are non-degenerate. That is, for every eigenvalue, there exists one linearly independent eigenvector.

Proof. Suppose ϕ_1, ϕ_2 are both solutions corresponding to the eigenvalue E. Then, we have

$$\begin{cases} \phi_1'' + k^2\phi_1 = 0, \\ \phi_2'' + k^2\phi_2 = 0, \end{cases}$$

where $k = \sqrt{\frac{2m}{\hbar^2}(E - V(x))}$. Thus, $\frac{\phi_1''}{\phi_1} = -k^2 = \frac{\phi_2''}{\phi_2}$, and so,

$$0 = \phi_1''\phi_2 - \phi_2''\phi_1 = \frac{\mathrm{d}}{\mathrm{d}x}((\phi_1'\phi_2) - (\phi_2'\phi_1)).$$

Integrating, we obtain $(\phi_1'\phi_2) - (\phi_2'\phi_1) = c$ for some $c \in \mathbb{C}$. But, as ϕ_1, ϕ_2 are bounded states, taking $x \to \infty$, we see that $c = 0$ and so $(\phi_1'\phi_2) - (\phi_2'\phi_1) = 0$. Finally, as this implies $\phi_1'/\phi_2 = \phi_2'/\phi_2$, integrating, we have $\ln \phi_1 = \ln \phi_2 + C$, and thus, $\phi_1 \propto \phi_2$. □

Proposition 4.5. Eigenfunctions in an even 1-dimensional potential are either even or odd functions.

Proof. See problem sheet. □

Proposition 4.6. The ground state (the eigenfunction with the lowest eigenenergy) does not have any zeros. Furthermore, the n-th excited state has n zeros inside the potiential.

4.2 Piecewise Constant Solutions