Mathematical Quantum Mechanics

MATH 470 Final Presentation

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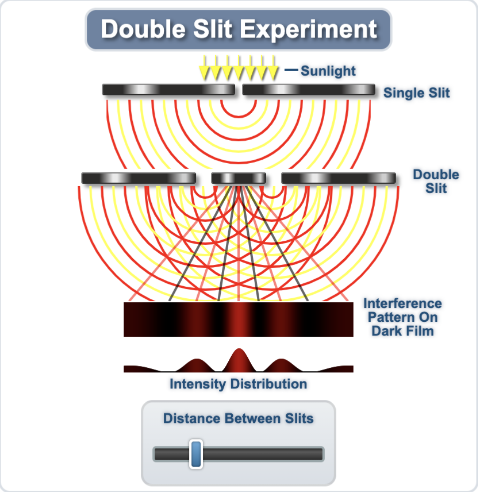
Introduction to Quantum Mechanics

- **Quantum Mechanics** is a theory of physics whereby quantities of a system, such as energy, momentum, and angular momentum, are restricted to taking on discrete quantities.
- Objects exhibit **wave-particle duality**
- **Uncertainty Principle**: Given a complete set of initial conditions, there are limits to how accurately we can predict values of certain physical quantities.

Historical Background

- **Late 1600s - early 1700s**: debate in the scientific community over the nature of light.
  - Newton (light is a group of particles) vs. Huygens (light is a wave).
- **1804:** Thomas Young's double slit experiment for light provided evidence for the *wave nature of light.*
- **1865:** Maxwell's equations predicted that EM waves would propagate at a certain speed which agreed with experimental observations.

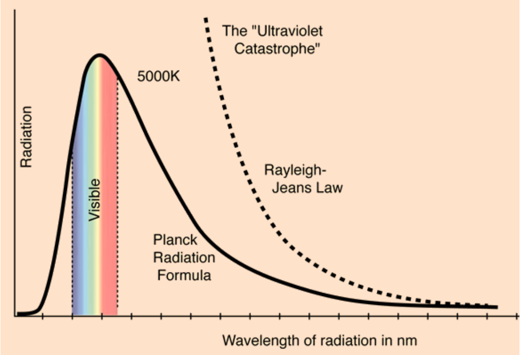
Consensus from 1865 - end of the 19th century:
light is a wave.



Historical Background

- **1900:** Planck's Model of Blackbody Radiation ⇒ rebirth of the particle theory of light.
  - **Equipartition Theorem of (classical) statistical mechanics**: results in the ultraviolet catastrophe.
  - Energy in the EM field at a frequency ω should be **quantized**.
- Einstein: EM energy at a given frequency comes in quanta with

$$E_{\text{quanta}} = h\nu. \tag{1}$$



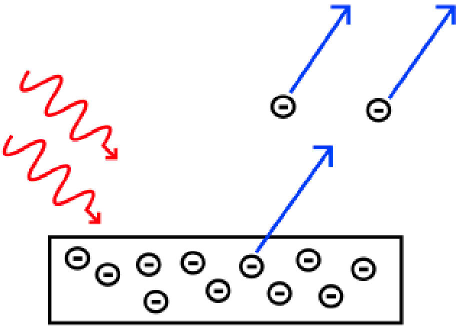
Historical Background

- **Photoelectric Effect (1921)**.
  - The particle theory of light explain the counter-intuitive experimental results. Each photon has energy $E = hf$, where $h = 6.63 \times 10^{-34} J \cdot s$.
- The phenomena of **wave-particle duality** was born.
- *Is an electron a wave or a particle?*
  - Spectrum of hydrogen: the energies of emitted photons when electrons jump between energy states can only come in certain discrete values:

$$E_n = -\frac{R}{n^2}, \text{ where } R = \frac{m_e Q^4}{2\hbar^2} \tag{2}$$

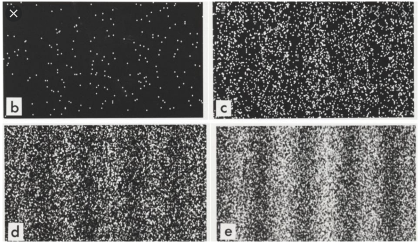
  - Observed frequencies:

$$\omega = \frac{1}{\hbar}(E_n - E_m) \text{ where } m > n \tag{3}$$



Historical Background

- **1989**: Distinctive interference pattern observed in the pattern of electron strikes.
- Schrödinger's 1926 papers provided the correct mathematical groundwork of QM; his *interpretation* is not that which is used.
    - Born (1926): statistical approach to QM. This approach is called the **Copenhagen interpretation of QM**.
- **Classical Mechanics**: given a particle of mass m subject to a force $F(\mathbf{x}, t)$, how do we determine $x(t)$ $\rightarrow$ Newton's 2nd Law.
- **Quantum Mechanics:** we want to obtain a **wave function** ψ which encodes the location and momentum of a particle. How do we determine $\psi(\mathbf{x}, t) \rightarrow$ Schrödinger's Eqn.



Mathematical Formulation of Classical Mechanics

Definition (Trajectory)

A solution $x(t)$ to Newton's Law, $F(x(t)) = ma = m\ddot{x}(t)$ where $m \geq 0$ is the mass of the particle, is called a **trajectory**.

- **Kinetic Energy**: $\frac{1}{2}mv^2$.
- **Potential Energy**:

$$V(x) := -\int F(x)dx. \tag{4}$$

  Total Energy: $E(x, v) := \frac{1}{2}mv^2 + V(x)$.
- The conservation of energy allows us to understand solutions to Newton's 2nd law. Reduce $F(x) = m\ddot{x}$ into a system of first order ODEs:

$$\frac{dx}{dt} = v(t) \qquad \frac{dv}{dt} = \frac{1}{m}F(x(t)). \tag{5}$$

Mathematical Formulation of Classical Mechanics

Using the conservation of energy, Newton's Second Law is reduced to the following first-order ODE:

$$\dot{x}(t) = \pm\sqrt{\frac{2(E_0 - V(x(t)))}{m}}. \tag{6}$$

Hamiltonian Approach to Classical Mechanics: we think of energy as a function of position and momentum rather than position ans velocity. Define the **Hamiltonian** of a particle in $\mathbb{R}^n$:

$$H(\mathbf{x}, \mathbf{p}) := \frac{1}{2m}\sum_{j=1}^{n} p_j^2 + V(\mathbf{x}). \tag{7}$$

Leads to **Hamilton's Equations**:

$$\frac{dx_j}{dt} = \frac{\partial H}{\partial p_j} \qquad \frac{dp_j}{dt} = -\frac{\partial H}{\partial x_j}. \tag{8}$$

Mathematical Formulation of Classical Mechanics

Definition (Poisson Bracket)

Let f, g be two smooth functions on $\mathbb{R}^{2n}$, where $(\mathbf{x}, \mathbf{p}) \in \mathbb{R}^{2n}$. Then, the **Poisson Bracket** of f and g, which we denote $\{f, g\}$, is a function on $\mathbb{R}^{2n}$ given by:

$$\{f, g\}(\mathbf{x}, \mathbf{p}) := \sum_{j=1}^{n} \left(\frac{\partial f}{\partial x_j} \frac{\partial g}{\partial p_j} - \frac{\partial f}{\partial p_j} \frac{\partial g}{\partial x_j} \right). \tag{9}$$

The Poisson Bracket is bi-linear and skew-symmetric, obeys a Leibniz rule, and obeys a **Jacobi Identity**:

$$\{f, \{g, h\}\} + \{h, \{f, g\}\} + \{g\{h, f\}\} = 0.$$

The position and momentum functions obey the following relations:

$$\{x_j, x_k\} = 0, \ \{p_j, p_k\} = 0, \ \{x_j, p_k\} = \delta_{jk}. \tag{10}$$

Mathematical Formulation of Classical Mechanics

- If $(\mathbf{x}(t), \mathbf{p}(t))$ solves Hamilton's equations, then for any smooth function f on $\mathbb{R}^{2n}$:

$$\frac{d}{dt} f(\mathbf{x}(t), \mathbf{p}(t)) = \{f, H\}(\mathbf{x}(t), \mathbf{p}(t)) \iff \frac{df}{dt} = \{f, H\}. \tag{11}$$

  - f is a conserved quantity $\iff$ $\{f, H\} = 0$. This implies H is a conserved quantity.
- Why does this help?
  - Using conserved quantities, or constants of motion, can reduce the numbers of dimensions for which we need to look for solutions.

Introduction to Quantum Mechanics

The deterministic description of a state in classical mechanics is replaced by a *probabilistic* description of a state in quantum mechanics.

1. These probabilities for the position are encoded in the square of the absolute value of the wave function $\psi(\mathbf{x}, t)$.
2. The probabilities for the momentum of a particle are encoded in the frequencies of the wave function.
3. Observables are described using operators.

The wave function, whose time-evolution is described by the **Schrödinger equation**, determines *statistical behaviour.*

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \left[-\frac{\hbar^2}{2m}\Delta + V(x,t)\right]\Psi(x,t). \tag{12}$$

We represent physical quantities such as position, momentum, and energy as operators on a Hilbert Space $\mathcal{H}$. We will assume that $\mathcal{H}$ is a Hilbert Space over $\mathbb{C}$ which is separable.

Preliminary Operator Theory

Our operators will in general be unbounded, analogous to classical mechanics. For physical and mathematical purposes, we will want our operators to be self-adjoint. Recall the adjoint:

$$\langle Ax, y\rangle = \langle x, A^* y\rangle. \tag{13}$$

- Recall: a linear operator A defined on all of such that $\langle \phi, A\psi\rangle = \langle A\phi, \psi\rangle \Rightarrow A$ bounded.
- **Unbounded Operator**: An unbounded operator A on $\mathcal{H}$ is a linear map from a dense subspace $\mathrm{Dom}(A) \subseteq \mathcal{H} \to \mathcal{H}$.

Definition (Adjoint)

Let A be an unbounded operator on $\mathcal{H}$. The **adjoint** A^* of A is defined as follows. A vector $\phi \in \mathcal{H}$ belongs to $\mathrm{Dom}(A^*)$ if the linear functional $\langle \phi, A\cdot\rangle$ is bounded on $\mathrm{Dom}(A)$. For $\phi \in \mathrm{Dom}(A^*)$, $A^*\phi$ is the unique vector v s.t. $\langle v, \psi\rangle = \langle \phi, A\psi\rangle$ for all $\psi \in \mathrm{Dom}(A)$.

Preliminary Operator Theory

- **Symmetric:** an unbounded operator A on $\mathcal{H}$ is **symmetric** if $\langle \phi, A\psi \rangle = \langle A\phi, \psi \rangle$ for all $\phi, \psi \in \mathrm{Dom}(A)$.
- **Self-Adjoint:** A is **self-adjoint** if $\mathrm{Dom}(A^*) = \mathrm{Dom}(A)$ and $A^*\phi = A\phi$ for all $\phi \in \mathrm{Dom}(A)$.
    - **Essentially self-adjoint:** A is **essentially self-adjoint** if the closure of the graph of A in $\mathcal{H} \times \mathcal{H}$ is the graph of a self-adjoint operator.
- Proofs of the following two claims are straightforward. If A is a symmetric operator on $\mathcal{H}$:
    1. If $\psi, A\psi, \ldots, A^{n-1}\psi \in \mathrm{Dom}(A)$, then $\langle \psi, A^n\psi \rangle \in \mathbb{R}$.
    2. If $A\psi = \lambda\psi$ for some $\psi \in \mathrm{Dom}(A) \setminus \{0\}$, then $\lambda \in \mathbb{R}$.

Physical meaning of $\langle \psi, A\psi \rangle$: this is the expected value for this measurement; λ is one of the potential outcomes. If A is self-adjoint, then the spectral theorem will give us a way to associate a probability measures to encode the probabilities for measurements of our observable in the state ψ.

Position and Momentum Operators

The probability that a particle's position is in a set $E \subseteq \mathbb{R}$ is:

$$\mathbb{P}[x \in E] = \int_E |\psi(x)|^2 dx. \tag{14}$$

For this probabilistic interpretation to make sense, we require that $||\psi||_{L^2} = 1$. For $m \geq 1$, the mth-**moment** of the position is what we'd expect:

$$\mathbb{E}[x^m] = \int_{\mathbb{R}} x^m |\psi(x)|^2 dx. \tag{15}$$

Key idea in QM: recasting expected values of physical quantities in terms of operators and inner products, so we can leverage the tools of functional analysis.

- **Position Operator**: $(X\psi)(x) := x\psi(x) \Rightarrow \mathbb{E}[x] = \langle \psi, X\psi \rangle$. Notation: $\langle X \rangle_\psi := \langle \psi, X\psi \rangle$.

Momentum Operator

Proposition. (de Broglie Hypothesis) If k is the spatial frequency of a particle's wave function, then the particle's momentum p is given by:

$$p = \hbar k. \tag{16}$$

Implies that $\psi(x) = e^{ikx}$ represents a particle with momentum $p = \hbar k$.

The functions $\frac{e^{ikx}}{\sqrt{2\pi}}, k \in \mathbb{Z}$ form an orthonormal basis for $L^2[0, 2\pi[$. A typical wave function for a particle on a circle is

$$\psi(x) = \sum_{k=-\infty}^{\infty} a_k \frac{e^{ikx}}{\sqrt{2\pi}}. \tag{17}$$

The expected value for the momentum is:

$$\mathbb{E}[p] = \sum_{k=-\infty}^{\infty} \hbar k |a_k|^2. \tag{18}$$

Momentum Operator

Imposing the condition that $\mathbb{E}[p^m] = \langle \psi, P^m \psi \rangle$. We see that P should satisfy $Pe^{ikx} = \hbar k e^{ikx}$. This leads to the following theorem.

Theorem (Momentum Operator)

Define the ***momentum operator*** *P by:*

$$P = -i\hbar \frac{d}{dx}. \tag{19}$$

Then, for all sufficiently nice $\psi \in L^2(\mathbb{R})$ s.t. $||\psi||_2 = 1$,

$$\langle \psi, P^m \psi \rangle = \int_{-\infty}^{\infty} (\hbar k)^m |\hat{\psi}(k)|^2 dk. \tag{20}$$

Math Detour: Fourier Transform

Meaning	**Fourier Series**	**Fourier Transform**
Weights	$a_k = \int_0^1 f(x)e^{-2\pi ikx}dx$	$\hat{f}(\xi) = \int_{-\infty}^{\infty} f(x)e^{-2\pi ix\xi}dx$
Function	$f(x) = \sum_{n=-\infty}^{\infty} a_n e^{2\pi inx}$	$f(x) = \int_{-\infty}^{\infty} \hat{f}(\xi)e^{2\pi ix\xi}d\xi$

Table: Fourier Transform v. Fourier Series

- A function f on $\mathbb{R}$ is said to be of **moderate decrease** if f is continuous and $\exists$ a $A > 0$ such that $|f(x)| \leq \frac{A}{1+x^2}$ for all $x \in \mathbb{R}$. The set of all functions of moderate decrease on $\mathbb{R}$ will be denoted by $\mathcal{M}(\mathbb{R})$.
- **Fourier Transform**: For $f \in \mathcal{M}(\mathbb{R})$, its **Fourier Transform** for $\xi \in \mathbb{R}$ is defined as:

$$\boxed{\hat{f}(\xi) := \int_{-\infty}^{\infty} f(x)e^{-2\pi ix\xi}dx} \tag{21}$$

Math Detour: Fourier Transform

- **Schwartz Space**: The **Schwartz Space** on $\mathbb{R}$, denoted $\mathcal{S}(\mathbb{R})$, is the set of all infinitely differentiable functions f for which all its derivatives are **rapidly decreasing**:

$$\sup_{x \in \mathbb{R}} |x|^k |f^{(\ell)}(x)| < \infty \text{ for all } k, \ell > 0. \tag{22}$$

  - Closed under standard operations, differentiation, and multiplication by polynomials.

Properties of the Fourier Transform for $f \in \mathcal{S}$. Let $h \in \mathbb{R}$ and $\delta > 0$.

1. $f(x+h) \to \hat{f}(\xi)e^{2\pi i h\xi}$.
2. $f(x)e^{-2\pi i x h} \to \hat{f}(\xi + h)$.
3. $f(\delta x) \to \delta^{-1}\hat{f}(\delta^{-1}\xi)$.
4. $f'(x) \to 2\pi i \xi \hat{f}(\xi)$.
5. $-2\pi i x f(x) \to \frac{d}{d\xi}\hat{f}(\xi)$.

Position and Momentum Operators

To summarize: the **position operator** X is defined by $X\psi(x) = x\psi(x)$ and the **momentum operator** P is defined by $P\psi(x) = -i\hbar\frac{d\psi}{dx}$. The crux of quantum mechanics is that P and Q do **NOT** commute.

Theorem (Canonical Commutation Relation)

The position and momentum operators X and P do not commute, but satisfy the relation:

$$XP - PX = i\hbar I. \tag{23}$$

- Note the parallel between the Poisson bracket relationship in classical mechanics $\{x, p\} = 1$ and the commutator of two operators A and B.
- X and P are symmetric operators on certain dense sub spaces of $L^2(\mathbb{R})$.

Axioms of Quantum Mechanics

1. **Axiom 1:** A system's state is represented by a unit vector ψ in a Hilbert space $\mathcal{H}$. If ψ_1 and ψ_2 are two unit vectors in $\mathcal{H}$ such that $\psi_2 = c\psi_1$ for $c \in \mathbb{C}$, then ψ_1 and ψ_2 represent the same physical state.
2. **Axiom 2:** Each real-valued function f (**classical observable**) on the *classical phase space* has a self-adjoint operator $\hat{f}$ (**quantum observable**) associated to it on the quantum Hilbert Space.
3. **Axiom 3:** If a quantum state is in a state described by a unit vector $\psi \in \mathcal{H}$, then the probability distribution corresponding to the measurement of an observable f satisfies:

$$\mathbb{E}[f^m] = \langle \psi, (\hat{f})^m \psi \rangle. \tag{24}$$

   3.1 By the self-adjointness of $\hat{f}$, the spectral theorem will provide a canonical way to construct a probability measure $\mu_{A,\psi}$ on $\mathbb{R}$.

Axioms of Quantum Mechanics

Theorem

Let $\psi \in \mathcal{H}$ be a unit vector describing a quantum system. If for some quantum observable $\hat{f}$ we have that $\hat{f}\psi = \lambda\psi$ for $\lambda \in \mathbb{R}$, then:

$$\mathbb{E}[f^m] = \langle (\hat{f})^m \rangle_\psi = \lambda^m. \tag{25}$$

for all $m \in \mathbb{N}$.

- The probability measure corresponding to this is the measure centred at λ. This is deterministic.
- When the state of a system is an *linear combination* of eigenvectors for $\hat{f}$, then the measurements of f will fail to be deterministic.
- For example, consider

$$\psi = \sum_{j=1}^{\infty} a_j e_j. \text{ Then, } \mathbb{P}[f = \lambda_j] = |a_j|^2. \tag{26}$$

Axioms of Quantum Mechanics

This leads us to our final kinematic axiom of quantum mechanics.

- **Axiom 4.** Suppose a quantum system is initially in a state ψ and that a measurement of an observable f is performed. If the result of the measurement is the number $\lambda \in \mathbb{R}$, then immediately after the measurement, the system will be in a state ψ' satisfying

$$\hat{f}\psi' = \lambda\psi'. \tag{27}$$

  We call this procedure the **collapse of the wave function**. The collapse of the wave function is a *discontinuous change in our knowledge of the state of the system.*

Uncertainty Principle

Theorem (Heisenberg's Uncertainty Principle)

Suppose $\psi \in \mathcal{S}$ is a unit vector in $L^2(\mathbb{R})$. Then,

$$\boxed{\left(\int_{-\infty}^{\infty} x^2 |\psi(x)|^2 dx\right)\left(\int_{-\infty}^{\infty} \xi^2 |\hat{\psi}(\xi)|^2 d\xi\right) \geq \frac{1}{16\pi^2}.} \tag{28}$$

Equality holds if and only if $\psi(x) = Ae^{-Bx^2}$, where $|A|^2 = \sqrt{2B/\pi}$.

Uncertainty Principle (Proof)

$$
\begin{aligned}
1 &= \int_{-\infty}^{\infty} |\psi(x)|^2 dx \\
&= -\int_{-\infty}^{\infty} x \frac{d}{dx} |\psi(x)|^2 dx \\
&= -\int_{-\infty}^{\infty} x \frac{d}{dx} [\psi(x)\psi^*(x)] dx \\
&= \left| -\int_{-\infty}^{\infty} x[\psi(x)(\psi^*(x))' + \psi'(x)\psi^*(x)] dx \right| \\
&\leq 2 \left(\int_{-\infty}^{\infty} |x\psi(x)|^2 dx \right)^{1/2} \left(\int_{-\infty}^{\infty} |x\psi'(x)|^2 dx \right)^{1/2}.
\end{aligned}
$$

Using Property 4 of the FT: $f'(x) \to 2\pi i \xi \hat{f}(\xi)$,

$$
\frac{1}{16\pi^2} \leq \left(\int_{-\infty}^{\infty} |x\psi(x)|^2 dx \right) \left(\int_{-\infty}^{\infty} |\xi\hat{\psi}(\xi)|^2 d\xi \right) \tag{29}
$$

Uncertainty Principle (Proof)

The **variance** is how we will quantify the uncertainty on our prediction of an observable:

$$\int_{-\infty}^{\infty} (x - \bar{x})^2 |\psi(x)|^2 dx. \tag{30}$$

By a simple change of variables, we get as a simple corollary of the Uncertainty Principle, the following bound on the simultaneous uncertainty of measuring the momentum and position of a particle:

$$\boxed{\frac{1}{16\pi^2} \leq \left(\int_{-\infty}^{\infty} (x - \bar{x})^2 |\psi(x)|^2 dx\right) \left(\int_{-\infty}^{\infty} (\xi - \bar{\xi})^2 |\hat{\psi}(\xi)|^2 d\xi\right)} \tag{31}$$

Time-Evolution

We can motivate the time-evolution QM using Planck's model of black-body radiation:

$$E = \hbar\omega. \tag{32}$$

Suppose ψ_0 has a definite energy E. Then, the state of the system at any other time t is:

$$\psi(t) = e^{-iEt/\hbar}\psi_0. \tag{33}$$

This leads to the following DE:

$$\frac{d\psi}{dt} = \frac{E}{i\hbar}\psi. \tag{34}$$

- **Axiom 5.** The time-evolution of the wave function ψ in a quantum system is given by the Schrödinger equation,

$$\frac{d\psi}{dt} = \frac{1}{i\hbar}\hat{H}\psi. \tag{35}$$

Time-Evolution

Theorem

Suppose $\psi(t)$ solve the Schrödinger Equation and A is a self-adjoint operator on $\mathcal{H}$. Then,

$$\frac{d}{dt}\langle A\rangle_{\psi(t)} = \left\langle \frac{1}{i\hbar}[A, \hat{H}] \right\rangle_{\psi(t)}. \tag{36}$$

- Classical mechanics analogue with the Poisson bracket.
  - For A, B self-adjoint operators,

$$(A, B) \mapsto \frac{1}{i\hbar}[A, B]. \tag{37}$$

- **Conserved quantities** occur when the operators commute; these are helpful in understanding how to solve Schrödinger's Equation.

Time-Independent Schrödinger Equation

Definition (Time-Independent Schrödinger Equation)

Let $\hat{H}$ be a Hamiltonian operator for a quantum system. Then, the **time-independent Schrödinger equation** is given by:

$$\hat{H}\psi = E\psi, \tag{38}$$

where $E \in \mathbb{R}$.

If ψ solves Equation 38, then

$$\psi(t) = e^{-itE/\hbar}\psi, \tag{39}$$

solves the *time-dependent* Schrödinger equation with initial data ψ.

Schrödinger Equation in $\mathbb{R}$

Based on the classical Hamiltonian for a particle,

$$\hat{H} = \frac{P^2}{2m} + V(X). \tag{40}$$

An operator of the following form is called a **Schrödinger Operator**:

$$\hat{H}\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x). \tag{41}$$

Given this, the **time-dependent Schrödinger equation** takes the form:

$$\boxed{\frac{\partial\psi(x,t)}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} - \frac{i}{\hbar}V(x)\psi(x,t).} \tag{42}$$

Time-Evolution of $\mathbb{E}[X]$ and $\mathbb{E}[P]$

Theorem

Suppose ψ solves the time-dependent Schrödinger equation. Suppose V and the initial condition $\psi(0) = \psi_0$ are nice. Then,

$$\frac{d}{dt}\langle X \rangle_{\psi(t)} = \frac{1}{m}\langle P \rangle_{\psi(t)} \tag{43}$$

$$\frac{d}{dt}\langle P \rangle_{\psi(t)} = -\langle V'(X) \rangle_{\psi(t)}. \tag{44}$$

- Similar to the classical case, except for the fact that there exist V such that

$$\langle V'(X) \rangle_{\psi} \neq V'(\langle X \rangle_{\psi}) \tag{45}$$

Spectral Theory

In the interest of time, I decided not to add this section since this talk is getting long. When I write the report, I'll include a brief write up on this section for those who are interested.

Thank you for listening!

References consulted in preparing this talk:

1. *Fourier Analysis: An Introduction* (Stein & Shakarchi).
2. *Quantum Theory for Mathematicians* (Hall).
3. *Mathematical Concepts of Quantum Mechanics* (Gustafson & Sigal).