PHYS 23410 (Quantum Mechanics I) Notes

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Weeks

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Week 1

Origins of Quantum Mechanics

1.1 Historical Perspective

- Intro to Wagner.
    - Will be teaching both Quantum I-II.
    - The structure of the course is explained in the syllabus on Canvas.
    - Every Friday, we get a new PSet due the next Friday.
        - This Friday, we will probably not get a PSet; PSet 1 will be handed out on Friday the 12th.
    - 50% of our grade is PSets; 50% is midterm and final.
        - This may fluctuate a bit.
    - Starting second week, we'll have 3 regular meetings each week.
    - If you have any problems, please get in touch with Wagner or the TAs!
    - Email: elcwagner@gmail.com.
    - OH will probably be on Wednesdays.
    - PSets posted on Canvas; solutions posted on Canvas after the deadline, too!
    - If there is something missing from Canvas, contact Wagner.
- Announcement.
    - No discussion sections today most likely; write to the TAs to confirm or if we want to discuss anything with the TAs.
    - Wagner will *hopefully* (not certainly) be back on Fridays.
- Outline of the course.
    1. Historical perspective.
        - Particle wave duality.
        - Uncertainty principle
    2. Schrödinger equation and the wave function.
    3. Formalism — observables in QM.
    4. Time-independent potentials.
        - One-dimensional problems.
    5. Angular momentum.
    6. Three dimensional problems.

- The hydrogen atom.

7. Spin, fermions, and bosons.

8. Symmetries and conservation laws.

- We now begin discussing the origins of quantum mechanics.

- **Photoelectric effect**: Electrons ejected from a metal when irradiated with light behave in a strange way.

  - In 1887, Hertz discovered this effect.
  - By 1905, it was clear that...
    1. No electrons were emitted unless the frequency of light was above a threshold value;
    2. The kinetic energy of the electrons grew linearly with frequency;
    3. The number of electrons depended on the light intensity.
  - These were three very strange phenomena.
  - In 1905, Einstein proposed a radical solution to this problem:
    1. Light is composed of **quanta**, that today we call **photons**.
    2. Each photon's energy is proportional to the frequency of light.
  - Essentially, Einstein said that if we model light this way, our model works.
  - Thus, the kinetic energy of the electrons is given by

$$K = h\nu - W$$

  where $h\nu$ is the kinetic energy of the photon and W is the minimum energy necessary to separate the electrons from the metal.

  - Assuming the intensity to be proportional to the number of photons, we obtain the right behavior.

- The constant that relates the energy of the photon to its frequency is

$$h = 6.626 \times 10^{-34}\,\mathrm{J\,s} = 4.125 \times 10^{-15}\,\mathrm{eV\,s}$$

and had been introduced before by Planck in 1900 to solve the so-called black body radiation problem.

  - Planck, however, thought of light emitted in quanta as a description of the emission process and not as the nature of light. In Planck's derivation, the average energy of the radiation emitted at a given frequency and temperature was given by a simple average weighted by Boltzmann factors:

$$\langle E \rangle = \frac{\sum nh\nu e^{-hn\nu/kT}}{\sum e^{-hn\nu/kT}} = \frac{h\nu}{e^{h\nu/kT} - 1}$$

    - $nh\nu$ is photon energy, and the e term is a Boltzmann factor.
    - Boltzmann factors won't play a further role in this course (phew!).
  - This implied a suppression for large frequencies instead of the classical value of kT. This value had been obtained for $h \to 0$, and it implied an unobserved infinite emission energy when summed over all frequencies!

- We now look into some implications of light quanta. Specifically, we will look at...

  - **Compton scattering**;
  - Light spectra;
  - Wave aspect of particles.

- **Compton scattering**:[1] The inelastic scattering of light off of a charged particle, resulting in a decrease in energy of the photon.
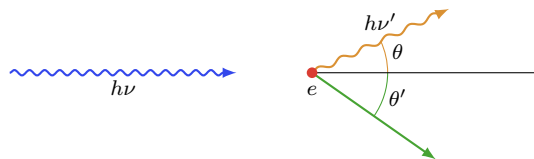

Figure 1.1: Compton scattering.

- – Further confirmation of the existence of quanta of light came from the study of its scattering with electrons.
  – Two properties were observed:
    1. Outgoing light had a different frequency than incoming.
    2. Frequency of the outgoing light depended on the emission angle.
  – Let's treat photons as relativistic particles. Conservation of energy and momentum should be imposed. Then we have...
    1. $h\nu + m_e c^2 = h\nu' + E_e$ — Energy.
    2. $h\nu = h\nu' \cos\theta + c|p_e|\cos\theta'$ — Momentum.
    3. $h\nu' \sin\theta = c|p_e|\sin\theta'$ — Momentum.
  – Where do these equations come from?
    ∎ Fact: $|p| = E/c$.
    ∎ Equations 2,3 have been multiplied through by c!
  – But we know that $E_e^2 = m_e^2 c^4 + c^2|p_e|^2$.
    ∎ "This should have been taught in a previous course." It wasn't for me. What else did I miss, and where can I read about it??
  – Hence, from (1),
$$(h\nu - h\nu' + m_e c^2)^2 = m_e^2 c^4 + c^2|p_e|^2$$
  – In addition, $(2)^2 + (3)^2$ yields
$$c^2|p_e|^2 = (h\nu - h\nu'\cos\theta)^2 + (h\nu'\sin\theta)^2$$
  – By substituting the second expression into the first, expanding, cancelling the common $m_e^2 c^4$, $(h\nu)^2$ and $(h\nu')^2$ factors on left and right, and algebraically rearranging, we get
$$2m_e c^2(h\nu - h\nu') = 2h^2\nu\nu'(1 - \cos\theta)$$
$$\frac{1}{\nu'} - \frac{1}{\nu} = \frac{h}{m_e c^2}(1 - \cos\theta)$$
  – This last result above is important!
  – Observe that we get $\nu = \nu'$ for $h = 0$; this is the classical result!
  – An alternate form of the above result may be obtained via the relation $c = \lambda\nu$:
$$\Delta\lambda = \lambda' - \lambda = \frac{h}{m_e c}(1 - \cos\theta)$$
  – The quantity $h/m_e c$ is called the **Compton wavelength** and plays an important role in atomic physics.

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[1]Recall the brief allusion to this in CHEM30200Notes.

  – Compton scattering experimental results are in full agreement with the light quanta predictions, i.e., the derivation just described!

- **Compton wavelength**: The quantity defined as follows. *Denoted by* $\boldsymbol{\lambda_c}$. *Given by*

$$\lambda_c = \frac{h}{m_e c} = 2.426 \times 10^{-12} \, \text{m}$$

- Light spectra.

  – From the definition of the Compton wavelength, we have that the energy of an electron is

$$E_e = m_e c^2 = \frac{ch}{\lambda_c} = 511 \, \text{keV}$$

  – Since gamma rays are those with $h\nu > 100 \, \text{keV}$, λ_c corresponds to one of these.
  – For comparison, visible light has a frequency of around $10^{15} \, \text{Hz}$, implying that $h\nu = 3 - 6 \, \text{eV}$

- Wave aspect of particles.

  – De Broglie, in 1923, speculated that since light behaved in a dual way (i.e., as a wave and also as a particle), so should any other particle in nature.
  – For instance, electrons must have a wave-light behavior.
  – Only difference between electrons and light is that electrons are massive (have mass), while light has a vanishing mass.
  – Light has energy $E = c|\vec{p}| = h\nu$ and momentum $\vec{p} = (h/2\pi) \cdot \vec{k}$, where $\vec{k}$ is the **wavevector** having magnitude $|\vec{k}| = 2\pi/\lambda$.
  – For massive particles,
$$E = \sqrt{c^2 \vec{p}^2 + m^2 c^4} = mc^2 \sqrt{1 + \frac{\vec{p}^2}{m^2 c^2}}$$

  – For nonrelativistic particles, $|\vec{p}| \ll mc$, so we may expand the square root's Taylor expansion to first order to get
$$E = mc^2 + \frac{\vec{p}^2}{2m}$$

    ■ Recall also that
$$\vec{p} = \hbar \vec{k}$$
    ■ Scalar-wise, note that $p = E/c = h\nu/c = h/\lambda = (h/2\pi)(2\pi/\lambda) = \hbar k$.
    ■ The derivation of angular momentum in the Bohr model yields the correct result (this one), even though the conceptual wave function used in the derivation is wrong.
    ■ Review these derivations and the relation to here!

  – It follows that
$$E - mc^2 = \frac{\vec{p}^2}{2m}$$
    where $E - mc^2$ is the kinetic energy
$$E_k = \hbar\omega$$

  – These assumptions lead to the form of the wave equation.

- **Wavevector**: The vector with magnitude equal to the wavenumber $2\pi/\lambda$ and direction perpendicular to the wavefront, that is, in the direction of wave propagation.

  – Wagner believes that this was covered in PHYS 13300; it wasn't.

- **Reduced Planck constant**: Planck's constant divided by 2π. *Denoted by $\hbar$. Given by*

$$\hbar = \frac{h}{2\pi}$$

- We now look into some implications of electrons being waves.

- The wave function for a free electron of momentum $\vec{p}$ will be

$$\psi_e \sim e^{i(\vec{k}\cdot\vec{r}-\omega t)}$$

where $\omega = 2\pi\nu$.

  - But if electrons are waves, then they can be represented in states that include the superposition of many wave functions.
  - Take two such waves $\psi_1(\vec{r},t)$ and $\psi_2(\vec{r},t)$.
  - Then

$$\psi = \alpha_1 e^{i(\vec{k}_1\vec{r}-\omega_1 t)} + \alpha_2 e^{i(\vec{k}_2\vec{r}-\omega_2 t)}$$

  is an acceptable electron wave function.

  - If we interpret $\hbar\vec{k}_1$ and $\hbar\vec{k}_2$ as momentum, we see an important difference between classical and quantum mechanics: The electrons may be *simultaneously in two different momentum states*.
  - Implication: There is in general no real "path" of the electron with a well-defined position and momentum. At most, one can define a "wave packet," with a certain mean value of position and momentum.

- How do we justify that electrons also behave like waves? With a double slit experiment, of course!

- Double slit experiment.

(a) Classical.   (b) Wave-mechanical.

Figure 1.2: Double slit experiment.

  - Let's take a beam of electrons impacting a wall with two slits.

    ■ Note that the focusing sheet with the single slit is not shown in Figure 1.2.
  - The electrons going through the slits are measured on a screen.
  - Classically, one expects the total number of electrons to be the simple sum of those going through slits $S1$ and $S2$.

    ■ If we cover one slit, we'll see one hump; if we cover the other slit, we'll see the other hump.
    ■ If both are uncovered, the humps will add to a big hump.
    ■ This is what's happening in Figure 1.2a.
  - If electrons behave as waves, however, the wave function $\psi = \psi_{S1} + \psi_{S2}$ will be the superpositions of the waves coming from $S1$ and $S2$.

    ■ $|\psi|^2 = I$ — next class, we will justify this, but for now we just accept it.
  - The intensity, proportional to the number of electrons, will be given by

$$|\psi|^2 = |\psi_{S1} + \psi_{S2}|^2 = |\psi_{S1}|^2 + |\psi_{S2}|^2 + (\psi_{S1}^*\psi_{S2} + \psi_{S2}^*\psi_{S1})$$

- Calling $I_i := |\psi_{Si}|^2$, the above equation transforms into

$$|\psi|^2 = I_1 + I_2 + 2\sqrt{I_1 I_2} \cos \delta$$

where δ is the phase difference that will depend on the waves' wavelength and the difference of the distances of the screens to the slits.

- We will therefore see an interference pattern.
- The observations are in full agreement with this prediction.

- What is this mysterious ψ?

- We know that $|\psi|^2$ is the density of probability of finding an electron in a given point.
- Essentially, if you take a small volume $\Delta V = \Delta x \Delta y \Delta z$, then $|\psi|^2 \Delta V$ is the probability of finding the electron in ΔV.
- Therefore, since the sum of all probabilities should be normalized to 1, we know that

$$\int_{-\infty}^{\infty} |\psi|^2 \, \mathrm{d}x \, \mathrm{d}y \, \mathrm{d}z = 1$$

- Typical lectures will be 100% blackboard-based, not this format.

- He will deliver notes at least one day before each lecture.

- Tell him if the lecture pace isn't good.

- Do the lectures align with the textbooks at all?

- Griffiths and Schroeter (2018) starts with the Schrödinger equation without motivation; Wagner doesn't like that, so he motivates it a bit and then goes with Griffiths and Schroeter (2018) from there.
- Some historical perspective is good.
  - UChicago used to have a course called Modern Physics that covered physics that was no longer modern to do all this stuff, but then they concluded it was useless and this content can be summarized in one lecture (today's!).
  - Nowadays, the optional QM III covers advanced topics.
- Most books (with rare exceptions) cover the same topics, so I can pretty much pick up any book I want to follow along with.
  - That being said, Landau and Lifshitz (1977) is far more advanced and not at all suitable for a first brush with the material, but it is beautiful and Wagner highly recommends it. Landau and Lifshitz (1977) provides great intuition.

1.2 The Wave Function and the Schrödinger Equation

1/5:
- Announcements.

- Largely reiterates from last time.
- 50-60% of the grade is related to PSet solutions.

- Last time:

- We talked about both light *and* particles as waves.
- We defined $\vec{p} = \hbar \vec{k}$ and $E = \vec{p}^2/2m = \hbar\omega$.

– The general form for a free wave is

$$\psi = A \exp\left[i(\vec{k} \cdot \vec{r} - \omega t)\right] = A \exp\left[\frac{i}{\hbar}(\vec{p} \cdot \vec{r} - Et)\right]$$

- If we evaluate $-i\hbar\vec{\nabla}\psi$ with ψ defined as above, then we get

$$-i\hbar\vec{\nabla}\psi = \vec{p}\psi$$

- In this course, we will denote differential operators with hats, e.g., the momentum operator is

$$\hat{\vec{p}} = -i\hbar\vec{\nabla}$$

- Observe that if we apply the momemtum operator twice, we obtain

$$(-i\hbar\vec{\nabla}) \cdot (-i\hbar\vec{\nabla}) = -\hbar^2\vec{\nabla}^2$$

– Recall that the gradient operator is defined via

$$\vec{\nabla} := \vec{x}\frac{\partial}{\partial x} + \vec{y}\frac{\partial}{\partial y} + \vec{z}\frac{\partial}{\partial z}$$

where $\vec{x}^{\,2} = \vec{y}^{\,2} = \vec{z}^{\,2} = 1$.

– Hence, by the definition of the dot product,

$$\vec{\nabla}^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

- Observe that if we evaluate $i\hbar\, \mathrm{d}\psi/\mathrm{d}t$ with ψ defined as above, then we get

$$i\hbar\frac{\mathrm{d}\psi}{\mathrm{d}t} = E\psi$$

- **Hamiltonian operator** (for a free particle): The operator defined as follows. *Denoted by $\hat{\boldsymbol{H}}$. Given by*

$$\hat{H} = \frac{\hat{\vec{p}}^{\,2}}{2m}$$

- Thus,

$$\hat{H}\psi = \frac{\vec{p}^{\,2}}{2m}\psi = \frac{p^2}{2m}\psi = E\psi = i\hbar\frac{\partial\psi}{\partial t}$$

which implies by transitivity that for a free particle,

$$\frac{\vec{p}^{\,2}}{2m}\psi = E\psi$$

- Recall that normally,

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

- Schrödinger postulated the **Schrödinger equation**.

- **Schrödinger equation**: The equation defined as follows. *Given by*

$$\hat{H}\psi = i\hbar\frac{\partial}{\partial t}\psi$$

$$-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi + V(\vec{r}, t)\psi = i\hbar\frac{\partial}{\partial t}\psi$$

- What do we know about ψ?

  - Recall from last time that

  $$\int_V |\psi|^2 \mathrm{d}^3\vec{r}$$

  represents the probability of finding the particle in the volume V.

  - In particular, this means that we must have

  $$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathrm{d}x \, \mathrm{d}y \, \mathrm{d}z \, |\psi|^2 = 1$$

- This greatly diverges from classical mechanics, where particles followed a well-defined path for which you could define a position and momentum at each point along the path.

- The Schrödinger equation has many nice properties. Examples:

  1. <u>Linearity part 1 (scalability)</u>: If ψ is a solution, then $k\psi$ is a solution where k is a constant.
     - This follows directly from the definition:

     $$-\frac{\hbar^2}{2m}\vec{\nabla}^2(k\psi) + V(\vec{r},t)k\psi = k\left[-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi + V(\vec{r},t)\psi\right] = k\left[i\hbar\frac{\partial}{\partial t}\psi\right] = i\hbar\frac{\partial}{\partial t}(k\psi)$$

  2. <u>Linearity part 2 (additivity)</u>: If ψ_1, ψ_2 are solutions, then $\psi_1 + \psi_2$ is a solution.
     - This is — once again — because of the linearity of the differential operators involved:

     $$\hat{H}(\psi_1 + \psi_2) = i\hbar\frac{\partial}{\partial t}(\psi_1 + \psi_2)$$

- Because of linearity, quantum mechanics is *easier* than classical mechanics in some sense.

- It follows from the two parts of linearity that if $\psi_1, \ldots, \psi_n$ are solutions and $c_1, \ldots, c_n$ are complex constants, then

$$\psi = \sum_{i=1}^{n} c_i \psi_i$$

  is a solution.

- What if I want to find the mean value of the *position* of the particle defined by ψ? Integrate over all space (I know that the particle will be somewhere there), and scale the probability of it being at each point by the distance to that point:

$$\langle \hat{\vec{r}} \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathrm{d}x \, \mathrm{d}y \, \mathrm{d}z \, |\psi(\vec{r},t)|^2 \vec{r}$$

  - Note that $\hat{\vec{r}} = \vec{r}$, i.e., the position operator is just the position!

- What if we want to find the mean value of the *momentum* of the particle defined by ψ? We have to do something less obvious:

$$\langle \hat{\vec{p}} \rangle = \int \mathrm{d}^3\vec{r} \, \psi^*(-i\hbar\vec{\nabla}\psi)$$

  - Is there a rationale for this construction??

- Why is it the mean value of the operator, not the quantity?

  - We will define the mean value of the quantity to be the mean value of the operator.

- Now let's relate mean momentum and position!

- Recall from classical mechanics that $\vec{p} = m \, \mathrm{d}\vec{r}/\mathrm{d}t$. Is there an analogy?

- Recall from E&M that $\partial \rho / \partial t + \vec{\nabla} \cdot \vec{J} = 0$; this is a relationship between density and current density.

- The analogous equation in quantum mechanics is

$$\frac{\partial |\psi|^2}{\partial t} + \vec{\nabla} \left[\frac{i\hbar}{2m} (\psi \vec{\nabla} \psi^* - \psi^* \vec{\nabla} \psi) \right] = 0$$

  ■ In PSet 1, we will derive this equation from from the Schrödinger equation by multiplying by ψ, ψ^* to the two sides and adding.

  ■ The derivation should be pretty straightforward.

- We now use this equation.

- Differentiate both sides of the $\langle \hat{\vec{r}} \rangle$ equation to get

$$\frac{\mathrm{d}\langle \hat{\vec{r}} \rangle}{\mathrm{d}t} = \int \mathrm{d}^3\vec{r} \; \vec{r} \frac{\partial}{\partial t} |\psi(\vec{r}, t)|^2$$
$$= \int \mathrm{d}^3\vec{r} \; \vec{r} \vec{\nabla} \left[-\frac{i\hbar}{2m} (\psi \vec{\nabla} \psi^* - \psi^* \vec{\nabla} \psi) \right]$$

- We now integrate by parts using

$$\int_{-\infty}^{\infty} \mathrm{d}x \, f(x) \cdot \frac{\mathrm{d}}{\mathrm{d}x} g(x) = \int_{-\infty}^{\infty} \mathrm{d}x \, \frac{\mathrm{d}}{\mathrm{d}x} [f(x) \cdot g(x)] - \int \mathrm{d}x \, g(x) \cdot \frac{\mathrm{d}}{\mathrm{d}x} f(x)$$

- In the three dimensional setting, we'll need the fact that

$$\frac{\partial}{\partial x_i} r_j = \delta_{ij}$$

  where δ denotes the Kronecker delta function.

- Thus, continuing from the above, we have that

$$\frac{\mathrm{d}\langle \hat{\vec{r}} \rangle}{\mathrm{d}t} = \int \mathrm{d}^3\vec{r} \; \left[\frac{i\hbar}{2m} \psi \vec{\nabla} \psi^* - \frac{i\hbar}{2m} \psi^* \vec{\nabla} \psi \right]$$
$$= \int \mathrm{d}^3\vec{r} \; \left[-\frac{i\hbar}{m} \psi^* \vec{\nabla} \psi \right]$$
$$= \frac{\langle \hat{\vec{p}} \rangle}{m}$$

- Ask about instances of notation changing.

- Note that in this course, ψ^* denotes the complex conjugate of ψ.

  - We don't use $\bar{\psi}$ here because bars often indicate something else in physics.

- Last note: All observables are real in quantum mechanics!

  - This is because all operators associated with quantum mechanics are **Hermitian**.

- **Hermitian** (operator): An operator satisfying the following equation. *Also known as* **self-adjoint**. *Constraint*

$$\int \mathrm{d}^3\vec{r} \; \psi^* \hat{O} \psi = \left(\int \mathrm{d}^3\vec{r} \; \psi \hat{O} \psi^* \right)^*$$

  - As with matrices, we have some kind of equality with the complex conjugate.

1.3   Chapter 0: Preface

From Griffiths and Schroeter (2018).

1/9:
- "Every competent physicist can 'do' quantum mechanics, but the stories we tell ourselves about what we are doing are as various" as can be (Griffiths & Schroeter, 2018, p. 11).

- "We do not believe one can intelligently discuss what quantum mechanics *means* until one has a firm sense of what quantum mechanics *does*," hence this book is devoted to teaching how to *do* quantum mechanics (Griffiths & Schroeter, 2018, p. 11).

- Mathematical prerequisites.

  - Legendre, Hermite, and Laguerre polynomials.
  - Spherical harmonics.
  - Bessel, Neumann, and Hankel functions.
  - Airy functions.
  - The Riemann zeta function.
  - Fourier transforms.
  - Hilbert spaces.
  - Hermitian operators.
  - Clebsch-Gordon coefficients.

- Griffiths and Schroeter (2018) recommend two math books for physicists that would explain the above concepts.

1.4   Chapter 1: The Wave Function

From Griffiths and Schroeter (2018).

- Section 1.1: The Schrödinger Equation.

- All systems that occur at the microscopic level are conservative!

- The setup in classical mechanics: Use Newton's second law to find a given particle's trajectory $x(t)$ and then derive any other quantity (e.g., v, p, T) that you want from there.

- The setup in quantum mechanics: Use the Schrödinger equation to find a given particle's wave function $\psi(x, t)$.

- Section 1.2: The Statistical Interpretation.

- **Statistical interpretation**: $|\psi(x,t)|^2$ gives the probability of finding the particle at the point x at time t.

  - Attributed to Max Born.

- Probability as the area under a curve.

- **Quantum indeterminacy**: Even if you know everything the theory has to tell you about a given particle (e.g., the theory tells you its wave function), still you cannot predict with certainty the outcome of a simple experiment to measure the particle's position.

- Is quantum indeterminacy a fact of nature or a defect in the theory?

  - Big physical/philosophical question!

- Suppose you measure the position of a given particle, finding that its at point C.

    - Where was the particle just before measuring?
    - Three plausible answers: The **realist**, **orthodox**, and **agnostic** positions.

- **Realist** (position): The particle was at C.

    - "The position of the particle was never indeterminate, but was merely unknown to the experimenter" (Griffiths & Schroeter, 2018, p. 17).
    - If this is true, then quantum mechanics is an **incomplete** theory, i.e., we are missing some **hidden variable** needed to prove a complete description of the particle.

- **Orthodox** (position): The particle wasn't really anywhere. *Also known as* **Copenhagen interpretation**.

    - Implication: It was the act of measurement that forced the particle to "take a stand."
    - Implication: "Observations not only *disturb* what is to be measured, they *produce* it... we *compel* [the particle] to assume a definite position" (Griffiths & Schroeter, 2018, p. 17).

- **Agnostic** (position): Refuse to answer.

    - Only way to establish where the particle was before moving is to take two measurements, but we can't do this physically.
    - Thus, why even worry about the question!

- John Bell in 1964 showed that there is an observable corresponding to whether the particle has a precise position prior to measurement, eliminating agnosticism and making the distinction between realism and orthodoxy a (mostly) experimental question.

    - The orthodox position is the most likely current contender following the experiment.

- Measuring position twice consecutively must give the same value.

    - We account for this by saying that the wave function **collapses** to a spike at C that we can measure again quickly before the wave function spreads out anew.

- Double slit experiment with electrons.

- Section 1.3: Probability.

- Largely a review of MathChapter B from CHEM26100Notes. A few important, novel things are noted below.

- Why do we measure spread via squared terms?

    - The most obvious way to measure spread would be to find out how far each individual is from the average via $\Delta j = j - \langle j \rangle$ and then compute $\langle \Delta j \rangle$. But $\langle \Delta j \rangle = 0$ always.
    - What else could we do? We could take the absolute value of Δj. But this would be computationally complicated and involve lots of signs of which to keep track.
    - Thus, we get around both the zeroing out problem and the sign problem by squaring to get $\langle (\Delta j)^2 \rangle$.

- **Probability density**: The proportionality factor $\rho(x)$ such that $\rho(x)\,\mathrm{d}x$ is the probability that an individual lies between x and $x + \mathrm{d}x$.

- Example 1.2: A really interesting continuous probability problem! Come back to if I have time.

- Section 1.4: Normalization.

- Recall that a wave function ψ is not necessarily normalized right off the bat, but since we have scalar linearity, we can normalize it!

- This also means that we neglect any trivial solutions ($\psi = 0, \infty$) as not corresponding to real particles, since these wavefunctions can't be normalized.

- "Physically realizable states correspond to the **square-integrable** solutions to Schrödinger's equation" (Griffiths & Schroeter, 2018, p. 29).

- If we only normalized ψ at $t = 0$, how do we know that it will stay normalized as ψ evolves?

  - It is a property of the Schrödinger equation that ψ does stay normalized.
  - Without this fact, the whole statistical interpretation would break down.

- Griffiths and Schroeter (2018) essentially answer PSet 1, Q1.

- Section 1.5: Momentum.

- **Expectation value**: The average of measurements on an ensemble of identically prepared systems.

  - The expectation value is *not* the average of repeated measurements of the same particle (because measurement changes the particle).

- We now justify why expectation values are calculated the way they are.

  - To begin, we have as in class that

$$\frac{\mathrm{d}\langle x \rangle}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\left(\int x|\psi|^2 \,\mathrm{d}x \right)$$

$$= \int x \frac{\partial}{\partial t}|\psi|^2 \,\mathrm{d}x$$

$$= \frac{i\hbar}{2m} \int x \frac{\partial}{\partial x}\left(\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi \right) \mathrm{d}x$$

We now invoke integration by parts. Let $u := x$ and $\mathrm{d}v := \partial/\partial x \, (\psi^* \, \partial\psi/\partial x - \partial\psi^*/\partial x \, \psi)\,\mathrm{d}x$. Then we obtain

$$= \frac{i\hbar}{2m}\left\{ \left[x\left(\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi \right) \right]_{-\infty}^{\infty} - \int \left(\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi \right) \mathrm{d}x \right\}$$

Since $\psi(\infty) = \psi^*(\infty) = \psi(-\infty) = \psi^*(-\infty) = 0$, the left term above goes to zero, leaving

$$= -\frac{i\hbar}{2m} \int \left(\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi \right) \mathrm{d}x$$

$$= -\frac{i\hbar}{2m}\left(\int \psi^* \frac{\partial \psi}{\partial x}\,\mathrm{d}x - \int \frac{\partial \psi^*}{\partial x}\psi \,\mathrm{d}x \right)$$

Now considering the right term above, let $u := \psi$ and $\mathrm{d}v := \partial\psi^*/\partial x \,\mathrm{d}x$. Then by both integration by parts and considering the behavior of ψ, ψ^* at $\pm\infty$ once again, we obtain

$$= -\frac{i\hbar}{2m}\left[\int \psi^* \frac{\partial \psi}{\partial x}\,\mathrm{d}x - \left([\psi\psi^*]_{-\infty}^{\infty} - \int \psi^* \frac{\partial \psi}{\partial x}\,\mathrm{d}x \right) \right]$$

$$= -\frac{i\hbar}{2m}\left[\int \psi^* \frac{\partial \psi}{\partial x}\,\mathrm{d}x - \left(0 - \int \psi^* \frac{\partial \psi}{\partial x}\,\mathrm{d}x \right) \right]$$

$$= -\frac{i\hbar}{2m}\left(\int \psi^* \frac{\partial \psi}{\partial x}\,\mathrm{d}x + \int \psi^* \frac{\partial \psi}{\partial x}\,\mathrm{d}x \right)$$

$$= -\frac{i\hbar}{m} \int \psi^* \frac{\partial \psi}{\partial x}\,\mathrm{d}x$$

- All integrals above are over all space.
- We use $\partial/\partial x$ instead of $\vec{\nabla}$ because the book is only treating the one-dimensional case so far; the two operators are entirely analogous, though, by the definition of $\vec{\nabla}$!

  – Aside: Interpreting the above result.

  - It is unclear that we could even give a well-defined conceptualization of the velocity $\langle v \rangle$ of a quantum particle.
  - It turns out that we can (see Chapter 3), but for now we will postulate that

$$\langle v \rangle := \frac{\mathrm{d}\langle x \rangle}{\mathrm{d}t}$$

  – It is much more customary to work with the *momentum* $\langle p \rangle = m\langle v \rangle$ of a quantum particle.

  – In terms of ψ, the above equation tells us that

$$\langle p \rangle = -i\hbar \int \psi^* \frac{\partial \psi}{\partial x} \, \mathrm{d}x$$

  – Let's rewrite the above expressions for $\langle x \rangle, \langle p \rangle$ in a more suggestive way.

$$\langle x \rangle = \int \psi^*[x]\psi \, \mathrm{d}x \qquad\qquad \langle p \rangle = \int \psi^*[-i\hbar(\partial/\partial x)]\psi \, \mathrm{d}x$$

  – Thus, we have derived expressions that we may call the **operators** representing position x and momentum p!

  – Fact: "All classical dynamical variables can be expressed in terms of position and momentum" (Griffiths & Schroeter, 2018, p. 33).

  - Example: $T = p^2/2m$.
  - Example: $\vec{L} = \vec{r} \times \vec{p}$.

  – Implication: To calculate the expectation value of any such quantity $Q(x,p)$, we simply replace every p by $-i\hbar(\partial/\partial x)$, insert the resulting operator between ψ^* and ψ, and integrate:

$$\langle Q(x,p) \rangle = \int \psi^*[Q(x, -i\hbar \, \partial/\partial x)]\psi \, \mathrm{d}x$$

  - In Chapter 3, we will put the above equation on firmer theoretical footing.

Week 2

The Schrödinger Equation

2.1 Ehrenfest Theorem and Uncertainty Principle

- Announcement: PSet 1 due Friday at midnight.

- Recap.

    - $\psi(\vec{r}, t)$ is a wave function to which we associate a **probability density**.

        ■ Integrating this probability density over a volume yields the probability that the particle is in V.

        ■ Moreover, ψ is not arbitrary but must satisfy the Schrödinger equation.

    - $\hat{\vec{p}}$ is the momentum operator, defined as the differential operator $-i\hbar\vec{\nabla}$.

    - Expressing the Schrödinger equation in terms of $\hat{\vec{p}}$, we see that it represents the application of a Hamiltonian operator in the usual form from last quarter (i.e., kinetic plus potential energy) to a certain function.

    - $\langle \hat{\vec{r}} \rangle$ is the mean position, and $\langle \hat{\vec{p}} \rangle$ is the mean momentum.

        ■ The mean position and mean momentum satisfy the classical relation, i.e., $\mathrm{d}\langle \hat{\vec{r}} \rangle \, / \, \mathrm{d}t = \langle \hat{\vec{p}} \rangle / m$.

- **Probability density**: The quantity given as follows. *Given by*

$$|\psi(\vec{r}, t)|^2$$

- We now prove something even more amazing than the classical relation result: An analogy to the classical Newton's law.

- **Ehrenfest's theorem**: The time derivative of the expectation value of the momentum operator is related to the expectation value of the force $F := -\vec{\nabla} V$ on a massive particle moving in a scalar potential $V(\vec{r}, t)$ as follows.

$$\frac{\mathrm{d}\langle \hat{\vec{p}} \rangle}{\mathrm{d}t} = \langle -\vec{\nabla} V(\vec{r}, t) \rangle$$

Proof. Consider the Schrödinger equation:

$$-i\hbar\frac{\partial \psi}{\partial t} = \frac{\hbar^2}{2m}\vec{\nabla}^2\psi - V(\vec{r}, t)\psi$$

Take the complex conjugate of it. This means that we're sending $i \mapsto -i$, keeping V fixed (it's real), and sending $\psi \mapsto \psi^*$ (the inclusion of i in the Schrödinger equation means that ψ is complex in general and thus has a nontrivial complex conjugate).

$$-i\hbar\frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m}\vec{\nabla}^2\psi^* + V(\vec{r}, t)\psi^*$$

We will use the above two equations to substitute into the following algebraic derivation.

$$\frac{\mathrm{d}\langle \hat{\vec{p}}\rangle}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\left(\int \mathrm{d}^3\vec{r}\,\psi^*(-i\hbar\vec{\nabla}\psi)\right)$$

$$= \int \mathrm{d}^3\vec{r}\,\frac{\partial \psi^*}{\partial t}(-i\hbar\vec{\nabla}\psi) + \int \mathrm{d}^3\vec{r}\,\psi^*\left(-i\hbar\vec{\nabla}\frac{\partial \psi}{\partial t}\right)$$

$$= \int \mathrm{d}^3\vec{r}\left[-i\hbar\frac{\partial \psi^*}{\partial t}(\vec{\nabla}\psi)\right] + \int \mathrm{d}^3\vec{r}\,\psi^*\vec{\nabla}\left(-i\hbar\frac{\partial \psi}{\partial t}\right)$$

$$= \int \mathrm{d}^3\vec{r}\left[-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi^*(\vec{\nabla}\psi)\right] + \int \mathrm{d}^3\vec{r}\,\psi^*\vec{\nabla}\left(\frac{\hbar^2}{2m}\vec{\nabla}^2\psi\right)$$

$$+ \int \mathrm{d}^3\vec{r}\left[V(\vec{r},t)\psi^*(\vec{\nabla}\psi) + \psi^*\vec{\nabla}(-V(\vec{r},t)\psi)\right]$$

$$= \int \mathrm{d}^3\vec{r}\,\psi^*\vec{\nabla}(-V(\vec{r},t)\psi)$$

$$= \int \mathrm{d}^3\vec{r}\,\psi^*(-\vec{\nabla}V(\vec{r},t))\psi$$

$$= \langle -\vec{\nabla}V(\vec{r},t)\rangle$$

as desired. $\square$

- How does everything cancel from the long line to the following line in the above proof??

- In quantum mechanics, we have **observables** which are in one-to-one correspondence with operators.

Observables	Operators ($\hat{O}$)
$\vec{r}$	$\hat{\vec{r}}$
$V(\vec{r},t)$	$\hat{V}(\vec{r},t)$
$\hat{\vec{p}}$	$-i\hbar\vec{\nabla}$
$\hat{H}$	$-\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{r},t)$

Table 2.1: Observables vs. operators.

  - Recall that any Hermitian operator has a real observable.

- Define
$$\hat{O}_{ij} := \int \mathrm{d}^3\vec{r}\,\psi_i^*\hat{O}\psi_j$$

  - Then note that
$$\hat{O}_{ij} = (\hat{O}_{ji})^*$$

  - Thus, an equivalent definition of a Hermitian operator is one such that the above equation is satisfied for all relevant i,j.

- Recall that the Schrödinger equation is linear.

  - Let $\psi = \sum_i c_i\psi_i$.
  - Then
$$\int \mathrm{d}^3\vec{r}\,\psi^*\hat{O}\psi = \sum_{i,j}\int \mathrm{d}^3\vec{r}\,c_i^*\psi_i^*\hat{O}c_j\psi_j = \sum_{i,j}c_i^*c_j\hat{O}_{ij}$$

is real.

– Takeaway: Averages over arbitrary wavefunctions are real.

– Similarly, suppose that $\vec{r}$ is Hermitian. Then any function $V(\vec{r})$ of it is also Hermitian.

– Once again,

$$\int \mathrm{d}^3\vec{r}\, \psi_i^*(-i\hbar\vec{\nabla}\psi_j) = \left(\int \mathrm{d}^3\vec{r}\, \psi_j^*(-i\hbar\vec{\nabla}\psi_i)\right)^* = \int \mathrm{d}^3\vec{r}\, \psi_j(i\hbar\vec{\nabla}\psi_i^*) \to -\int \mathrm{d}^3\vec{r}\, \vec{\nabla}\psi_j(i\hbar\psi_i^*)$$

Involves integration by parts?? Perhaps via

$$\int \mathrm{d}^3\vec{r}\, \psi_j(i\hbar\vec{\nabla}\psi_i^*) = i\hbar \int \mathrm{d}^3\vec{r}\, \vec{\nabla}(\psi_j\psi_i^*) - \int \mathrm{d}^3\vec{r}\, \vec{\nabla}\psi_j(i\hbar\psi_i^*)$$

$$= i\hbar\vec{\nabla} \int \mathrm{d}^3\vec{r}\, (\psi_j\psi_i^*) - \int \mathrm{d}^3\vec{r}\, \vec{\nabla}\psi_j(i\hbar\psi_i^*)$$

$$= i\hbar\vec{\nabla}0 - \int \mathrm{d}^3\vec{r}\, \vec{\nabla}\psi_j(i\hbar\psi_i^*)$$

$$= -\int \mathrm{d}^3\vec{r}\, \vec{\nabla}\psi_j(i\hbar\psi_i^*)$$

What is the takeaway??

• Linear algebra analogy.

– Recall that we can write any vector $\vec{v}$ componentwise as $\vec{v} = v_x\vec{x} + v_y\vec{y} + v_z\vec{z}$.

– We can apply matrices A to such vectors to generate other vectors via $A\vec{v} = \vec{v}'$ and the like.

– Lastly, we have an inner product $\cdot$ such that $\vec{a} \cdot \vec{b} = \delta_{ab}$, where $a, b = x, y, z$.

– On an infinite-dimensional vector space, such as that containing all the ψ, we still can decompose $\psi = \sum_n c_n\psi_n$ into an infinite sum of basis components, apply operators $\hat{O}\psi = \psi'$, and have an inner product $\int \mathrm{d}^3\vec{r}\, \psi_m^*\psi_n = \delta_{mn}$.

– Another analogy: Like the inner product of a vector and unit vector is the component of the vector in that direction (e.g., $\vec{v} \cdot \vec{x} = v_x$), we have

$$\int \mathrm{d}^3\vec{r}\, \psi_m^*\psi = \int \mathrm{d}^3\vec{r}\psi_m^* \sum_n c_n\psi_n = c_m$$

– One more analogy: $\vec{x}^T A\vec{x} = A_{xx}$ is like $\langle\psi_i|\hat{O}|\psi_i\rangle = \hat{O}_{ii}$.

2.2 Time-Independent Potentials

1/10:   • Recap of important equations.

– Momentum and Hamiltonian operators.

– Schrödinger equation.

– Expectation values of $\vec{x}$ and $\vec{p}$, the classical relation between them, and Ehrenfest's theorem.

– Hermitian operator condition.

■ The fact that their observables are real.

■ Examples: $\hat{\vec{p}}$, $\hat{H}$, $\hat{\vec{p}}^2/2m$, $V(\vec{r}, t)$.

• **Adjoint** (of $\hat{O}$): The operator defined according to the following rule. *Denoted by* $\hat{\boldsymbol{O}}^\dagger$. *Constraint*

$$\int \mathrm{d}^3\vec{r}\, \psi_i^*\hat{O}\psi_j = \int \mathrm{d}^3\vec{r}\, (\hat{O}^\dagger\psi_i)^*\psi_j$$

– A self-adjoint (Hermitian) operator is an operator satisfying $\hat{O} = \hat{O}^\dagger$.

- Dirac notation.

  - Associate with each $\psi(\vec{r}, t)$ a "ket" $|\psi\rangle$ and a "bra" $\langle\psi|$.

    ■ These are like vectors.

  - The full "bra-ket" $\langle\psi_i|\psi_j\rangle := \int \mathrm{d}^3\vec{r}\ \psi_i^*\psi_j$.

  - We also have $\langle\psi_i|\hat{O}|\psi_j\rangle := \int \mathrm{d}^3\vec{r}\ \psi_i^*\hat{O}\psi_j$.

- The condition for an operator being Hermitian/self-adjoint in Dirac notation:

$$\langle\psi_i|\hat{O}|\psi_j\rangle = \left\langle\psi_i\middle|\hat{O}\psi_j\right\rangle = \left\langle\hat{O}^\dagger\psi_i\middle|\psi_j\right\rangle$$

- We also have that

$$\langle\psi_i|\hat{O}_1\hat{O}_2|\psi_j\rangle = \left\langle\psi_i\middle|\hat{O}_1\hat{O}_2\psi_j\right\rangle = \left\langle\hat{O}_1^\dagger\psi_i\middle|\hat{O}_2\psi_j\right\rangle = \left\langle\hat{O}_2^\dagger\hat{O}_1^\dagger\psi_i\middle|\psi_j\right\rangle$$

  - This is very relevant to PSet 1, Q3a!

- Dirac notation allows us to represent complicated expressions such as

$$\int \mathrm{d}^3\vec{r}\ {\psi'}^*\psi = \left(\int \mathrm{d}^3\vec{r}\ \psi^*\psi'\right)^*$$

  in the form

$$\langle\psi|\psi'\rangle = \left(\langle\psi'|\psi\rangle\right)^*$$

- In Dirac notation, the Hermitian condition becomes

$$\left\langle\psi_i\middle|\hat{O}_1\hat{O}_2\psi_j\right\rangle = \left\langle\hat{O}_2\hat{O}_1\psi_i\middle|\psi_j\right\rangle$$

- We also have that

$$\left\langle\psi_i\middle|\hat{O}_1\hat{O}_2\psi_j\right\rangle = \left(\left\langle\psi_j\middle|\hat{O}_2\hat{O}_1\psi_i\right\rangle\right)^*$$

  - This is also relevant to PSet 1, Q3a!

- This last statement has some consequences.

  - In particular, if $\psi_i = \psi_j = \psi$, then

$$\left\langle\psi\middle|\hat{O}_1\hat{O}_2\psi\right\rangle = \left(\left\langle\psi\middle|\hat{O}_2\hat{O}_1\psi\right\rangle\right)^*$$

  - Thus, by adding and subtracting the quantities in the above result, we learn that

$$\left\langle\psi\middle|(\hat{O}_1\hat{O}_2 - \hat{O}_2\hat{O}_1)\psi\right\rangle$$

  is an imaginary number and

$$\left\langle\psi\middle|(\hat{O}_1\hat{O}_2 + \hat{O}_2\hat{O}_1)\psi\right\rangle$$

  is a real number.

- Example: The commutator of the position and momentum operators gives a purely imaginary number.

  - We have that

$$[\hat{\vec{p}}_x, \hat{x}]f = (\hat{\vec{p}}_x x - x\hat{\vec{p}}_x)f = -i\hbar\frac{\partial}{\partial x}(xf) + xi\hbar\frac{\partial f}{\partial x} = -i\hbar\frac{\partial x}{\partial x}f - i\hbar x\frac{\partial f}{\partial x} + i\hbar x\frac{\partial f}{\partial x} = -i\hbar f$$

– Thus,
$$[\hat{\vec{p}}_x, \hat{x}] = -i\hbar$$
as desired.

- Can ψ_n be an eigenstate of $\hat{O}_1$ and $\hat{O}_2$ simultaneously?

  – In the mold of a typical eigenvalue equation $A\vec{x}_n = \lambda_n\vec{x}_n$, let
  $$\hat{O}\psi_n = O_n\psi_n \qquad\qquad \hat{O}_1\psi_n = O_{1,n}\psi_n \qquad\qquad \hat{O}_2\psi'_m = O_{2,m}\psi'_m$$

  – Then we have that
  $$\hat{O}_1\psi_n = O_{1,n}\psi_n$$
  $$\hat{O}_2\hat{O}_1\psi_n = O_{1,n}\hat{O}_2\psi_n = O_{1,n}O_{2,n}\psi_n$$
  and
  $$\hat{O}_2\psi_n = O_{2,n}\psi_n$$
  $$\hat{O}_1\hat{O}_2\psi_n = O_{2,n}\hat{O}_1\psi_n = O_{2,n}O_{1,n}\psi_n$$

  – These are the relevant constraints.
  – If such a ψ_n exists, then we can determine the values of $\hat{O}_1, \hat{O}_2$ simultaneously to infinite precision.

- The commutator is associated with a compatible observable.

  – In particular, when two operators commute, we say that the associated physical observables are **compatible**.

- Because waves move in a **wave packet**, there is some uncertainty in the position.

  – In particular, the uncertainty of $\hat{A}$ in a given state ψ is
  $$\langle\psi|(\hat{A} - \langle\hat{A}\rangle)^2|\psi\rangle$$

  – An alternate form of this expression is
  $$\langle\psi|\langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2|\psi\rangle$$

    ■ Wagner proves this as in MathChapter B from CHEM26100Notes.

- **Wave packet**: It is a continuous sum of waves of different frequencies.

- If ψ_n is an eigenstate of $\hat{A}$...

  – Then
  $$\langle\psi_n|\hat{A}|\psi_n\rangle = A_n\langle\psi_n|\psi_n\rangle = A_n$$
  – Similarly,
  $$\langle\psi_n|\hat{A}^2|\psi_n\rangle = A_n^2\langle\psi_n|\psi_n\rangle = A_n^2$$
  – Therefore, the uncertainty of $\hat{A}$ in an eigenstate is $A_n^2 - (A_n)^2 = 0$.

- Note that the condition "ψ is an eigenstate of $\hat{A}$" can be denoted via $\hat{A}|\psi_n\rangle = A_n|\psi_n\rangle$.

- **Heisenberg uncertainty principle**. *Given by*
$$\sigma_x\sigma_{p_x} \geq \frac{\hbar}{2}$$

- Why is this the case? It is related to $[p_x, x] = -i\hbar$.

  – The full derivation is in the notes (transcribed below), but for now, know that it is a general fact that

  $$\sigma_A^2 \sigma_B^2 \geq \frac{1}{4} |\langle \psi | [A, B] | \psi \rangle|^2$$

  – We demonstrate this via the **Schwarz inequality**.

  – One thing is always complex; the other is always real.

- **Cauchy-Schwarz inequality**. *Given by*

  $$(f, f)(g, g) \geq |(f, g)|^2$$

  – (f, g) denotes the inner product of f and g, where f, g are elements of an abstract vector space.

- **Schwarz inequality**. *Given by*

  $$\left(\int \mathrm{d}^3 \vec{r} \, |f|^2 \right) \left(\int \mathrm{d}^3 \vec{r} \, |g|^2 \right) \geq \left| \int \mathrm{d}^3 \vec{r} \, fg^* \right|^2$$

  – In Dirac's notation, this is

  $$\langle f | f \rangle \cdot \langle g | g \rangle \geq |\langle f | g \rangle|^2$$

- Full derivation of the Heisenberg uncertainty principle.

  – Apply the Schwarz inequality to $f = (\hat{A} - \langle \hat{A} \rangle) \psi$ and $g = (\hat{B} - \langle \hat{B} \rangle) \psi$, for $\hat{A}, \hat{B}$ Hermitian.

  – Recall that the following identities hold for Hermitian/self-adjoint operators.

  $$\langle \psi | \hat{A} | \psi' \rangle = \left\langle \psi \middle| \hat{A} \psi' \right\rangle = \left\langle \hat{A} \psi \middle| \psi' \right\rangle \qquad\qquad \langle \psi | \hat{A}^2 | \psi' \rangle = \left\langle \hat{A} \psi \middle| \hat{A} \psi' \right\rangle$$

  – Consequently, we have that

  $$\begin{aligned}
  \sigma_A^2 \cdot \sigma_B^2 &= \langle \psi | (\hat{A} - \langle \hat{A} \rangle)^2 | \psi \rangle \cdot \langle \psi | (\hat{B} - \langle \hat{B} \rangle)^2 | \psi \rangle \\
  &= \left\langle (\hat{A} - \langle \hat{A} \rangle) \psi \middle| (\hat{A} - \langle \hat{A} \rangle) \psi \right\rangle \cdot \left\langle (\hat{B} - \langle \hat{B} \rangle) \psi \middle| (\hat{B} - \langle \hat{B} \rangle) \psi \right\rangle \\
  &\geq \left| \left\langle (\hat{A} - \langle \hat{A} \rangle) \psi \middle| (\hat{B} - \langle \hat{B} \rangle) \psi \right\rangle \right|^2 \\
  &= \left| \langle \psi | \underbrace{(\hat{A} - \langle \hat{A} \rangle)}_{\Delta \hat{A}} \underbrace{(\hat{B} - \langle \hat{B} \rangle)}_{\Delta \hat{B}} | \psi \rangle \right|^2
  \end{aligned}$$

  Now, any product of operators can be expressed as one half of the sum of the **commutator** and the **anticommutator**. Thus, continuing,

  $$\begin{aligned}
  &= \left| \langle \psi | \frac{1}{2} ([\Delta \hat{A}, \Delta \hat{B}] + \{\Delta \hat{A}, \Delta \hat{B}\}) | \psi \rangle \right|^2 \\
  &= \frac{1}{4} \left| \langle \psi | [\Delta \hat{A}, \Delta \hat{B}] + \{\Delta \hat{A}, \Delta \hat{B}\} | \psi \rangle \right|^2
  \end{aligned}$$

  Recall from above that the mean value of the commutator is an imaginary number and the mean value of the anticommutator is a real number. Thus, if we split the above equation into two terms, the mean value of the anticommutator will be squared, hence a positive number that we can get rid of and maintain the inequality. Lastly, we can compute that $[\Delta \hat{A}, \Delta \hat{B}] = [\hat{A}, \hat{B}]$. Therefore,

  $$\geq \frac{1}{4} \left| \langle \psi | [\hat{A}, \hat{B}] | \psi \rangle \right|^2$$

- Example: Since $[p_x, x] = -i\hbar$, we can recover the Heisenberg uncertainty principle from the above inequality.
- There's some stuff in the notes that is very relevant to PSet 1, Q3b.

- **Commutator** (of $\hat{O}_1, \hat{O}_2$): The operator defined as follows. *Denoted by* $[\hat{\boldsymbol{O}}_{\mathbf{1}}, \hat{\boldsymbol{O}}_{\mathbf{2}}]$. *Given by*

$$[\hat{O}_1, \hat{O}_2] = \hat{O}_1 \hat{O}_2 - \hat{O}_1 \hat{O}_2$$

- **Anticommutator** (of $\hat{O}_1, \hat{O}_2$): The operator defined as follows. *Denoted by* $\{\hat{\boldsymbol{O}}_{\mathbf{1}}, \hat{\boldsymbol{O}}_{\mathbf{2}}\}$. *Given by*

$$\{\hat{O}_1, \hat{O}_2\} = \hat{O}_1 \hat{O}_2 + \hat{O}_2 \hat{O}_1$$

2.3 Office Hours (Matt)

- PSet1, Q2a: Conceptual reason why the first term in the integration by parts vanishes?
  - Boundary conditions in each of the three directional integrals.
- Quite heavily attended, but Matt still got around.

References

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Landau, L. D., & Lifshitz, E. M. (1977). *Qauntum mechanics: Non-relativistic theory* (Third). Elsevier Butterworth-Heinemann.