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

1/3:
- 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:

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

    - $nh\nu$ 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.

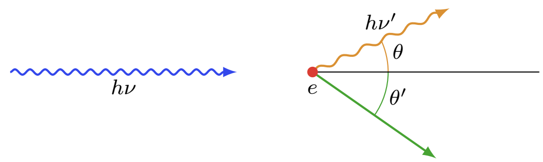


Figure 1.1: Compton scattering.

  - 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. $h\nu + m_ec^2 = h\nu' + E_e$ — 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 $E_e^2 = m_e^2c^4 + c^2|p_e|^2$.
    - "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),
$$(h\nu - h\nu' + m_ec^2)^2 = m_e^2c^4 + c^2|p_e|^2$$
  - 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 $m_e^2c^4$, $(h\nu)^2$ and $(h\nu')^2$ factors on left and right, and algebraically rearranging, we get
$$2m_ec^2(h\nu - h\nu') = 2h^2\nu\nu'(1-\cos\theta)$$
$$\frac{1}{\nu'} - \frac{1}{\nu} = \frac{h}{m_ec^2}(1-\cos\theta)$$
  - 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 $c = \lambda\nu$:
$$\Delta\lambda = \lambda' - \lambda = \frac{h}{m_ec}(1-\cos\theta)$$
  - The quantity h/m_ec is called the **Compton wavelength** and plays an important role in atomic physics.

[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,

$$E = \sqrt{c^2\vec{p}^2 + m^2c^4} = mc^2\sqrt{1 + \frac{\vec{p}^2}{m^2c^2}}$$

  - 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* $\boldsymbol{\hbar}$. *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

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

  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

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

    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. *Also known as* **time-dependent Schrödinger equation**, **TDSE**. *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. Linearity part 1 (scalability): 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. Linearity part 2 (additivity): 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 $\psi_1, \dots, \psi_n$ are solutions and $c_1, \dots, c_n$ 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

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

- 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

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

- 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

$$\begin{aligned}\frac{\mathrm{d}\langle x\rangle}{\mathrm{d}t} &= \frac{\mathrm{d}}{\mathrm{d}t}\left(\int x|\psi|^2\,\mathrm{d}x\right)\\ &= \int x\frac{\partial}{\partial t}|\psi|^2\,\mathrm{d}x\\ &= \frac{i\hbar}{2m}\int x\frac{\partial}{\partial x}\left(\psi^*\frac{\partial\psi}{\partial x}-\frac{\partial\psi^*}{\partial x}\psi\right)\mathrm{d}x\end{aligned}$$

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

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

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

$$\begin{aligned}&= -\frac{i\hbar}{2m}\left[\int\psi^*\frac{\partial\psi}{\partial x}\,\mathrm{d}x - \left([\psi\psi^*]_{-\infty}^{\infty} - \int\psi^*\frac{\partial\psi}{\partial x}\,\mathrm{d}x\right)\right]\\ &= -\frac{i\hbar}{2m}\left[\int\psi^*\frac{\partial\psi}{\partial x}\,\mathrm{d}x - \left(0 - \int\psi^*\frac{\partial\psi}{\partial x}\,\mathrm{d}x\right)\right]\\ &= -\frac{i\hbar}{2m}\left(\int\psi^*\frac{\partial\psi}{\partial x}\,\mathrm{d}x + \int\psi^*\frac{\partial\psi}{\partial x}\,\mathrm{d}x\right)\\ &= -\frac{i\hbar}{m}\int\psi^*\frac{\partial\psi}{\partial x}\,\mathrm{d}x\end{aligned}$$

- 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

1/8:

- 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).

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

Also observe that

$$\int \mathrm{d}^3\vec{r}\ \psi^*\vec{\nabla}(\vec{\nabla}^2\psi) = \int \mathrm{d}^3\vec{r}\ \vec{\nabla}\cdot[\psi^*\vec{\nabla}^2\psi] - \int \mathrm{d}^3\vec{r}\ \vec{\nabla}\psi^*\vec{\nabla}^2\psi = -\int \mathrm{d}^3\vec{r}\ \vec{\nabla}\psi^*\vec{\nabla}^2\psi$$

where the first term goes to zero by the divergence theorem and the boundary condition. (See PSet 1, Q2a for a full explanation of this zeroing out.) Similarly, we have that

$$\int \mathrm{d}^3\vec{r}\ \vec{\nabla}\psi^*\vec{\nabla}(\vec{\nabla}\psi) = -\int \mathrm{d}^3\vec{r}\ \vec{\nabla}^2\psi^*\vec{\nabla}\psi$$

This means that altogether,

$$\begin{aligned}\int \mathrm{d}^3\vec{r}\ \psi^*\vec{\nabla}^3\psi &= \int \mathrm{d}^3\vec{r}\ \vec{\nabla}^2\psi^*\vec{\nabla}\psi\\ \int \mathrm{d}^3\vec{r}\ [\vec{\nabla}^2\psi^*\vec{\nabla}\psi - \psi^*\vec{\nabla}^3\psi] &= 0\end{aligned}$$

We will now use the two Schrödinger substitutions and the above equation to substitute into the following algebraic derivation.

$$\begin{aligned}\frac{\mathrm{d}\langle\hat{\vec{p}}\rangle}{\mathrm{d}t} &= \frac{\mathrm{d}}{\mathrm{d}t}\left(\int \mathrm{d}^3\vec{r}\ \psi^*(-i\hbar\vec{\nabla}\psi)\right)\\
&= \int \mathrm{d}^3\vec{r}\ \frac{\partial\psi^*}{\partial t}(-i\hbar\vec{\nabla}\psi) + \int \mathrm{d}^3\vec{r}\ \psi^*\left(-i\hbar\vec{\nabla}\frac{\partial\psi}{\partial t}\right)\\
&= \int \mathrm{d}^3\vec{r}\left(-i\hbar\frac{\partial\psi^*}{\partial t}\right)(\vec{\nabla}\psi) + \int \mathrm{d}^3\vec{r}\ \psi^*\vec{\nabla}\left(-i\hbar\frac{\partial\psi}{\partial t}\right)\\
&= \int \mathrm{d}^3\vec{r}\left(-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi^* + V(\vec{r},t)\psi^*\right)(\vec{\nabla}\psi)\\
&\quad + \int \mathrm{d}^3\vec{r}\ \psi^*\vec{\nabla}\left(\frac{\hbar^2}{2m}\vec{\nabla}^2\psi - V(\vec{r},t)\psi\right)\\
&= \int \mathrm{d}^3\vec{r}\left[-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi^*(\vec{\nabla}\psi)\right] + \int \mathrm{d}^3\vec{r}\ \psi^*\vec{\nabla}\left(\frac{\hbar^2}{2m}\vec{\nabla}^2\psi\right)\\
&\quad + \int \mathrm{d}^3\vec{r}\left[V(\vec{r},t)\psi^*(\vec{\nabla}\psi) + \psi^*\vec{\nabla}[-V(\vec{r},t)\psi]\right]\\
&= \int \mathrm{d}^3\vec{r}\ -\frac{\hbar^2}{2m}\left[\vec{\nabla}^2\psi^*(\vec{\nabla}\psi) - \psi^*\vec{\nabla}^3\psi\right]\\
&\quad + \int \mathrm{d}^3\vec{r}\left[V(\vec{r},t)\psi^*(\vec{\nabla}\psi) - \psi^*\vec{\nabla}[V(\vec{r},t)]\psi - \psi^*V(\vec{r},t)(\vec{\nabla}\psi)\right]\\
&= \int \mathrm{d}^3\vec{r}\ \psi^*(-\vec{\nabla}V(\vec{r},t))\psi\\
&= \langle-\vec{\nabla}V(\vec{r},t)\rangle\end{aligned}$$

as desired. □

- 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.
  - For example, the momentum operator is a Hermitian operator:
$$\int \mathrm{d}^3\vec{r}\ \psi_i^*(-i\hbar\vec{\nabla}\psi_j) = \left(\int \mathrm{d}^3\vec{r}\ \psi_j^*(-i\hbar\vec{\nabla}\psi_i)\right)^* = \int \mathrm{d}^3\vec{r}\ \psi_j(i\hbar\vec{\nabla}\psi_i^*) \to -\int \mathrm{d}^3\vec{r}\ \vec{\nabla}\psi_j(i\hbar\psi_i^*)$$
  - To prove the leftmost equality above, we can use integration by parts as follows.
$$\begin{aligned}\int \mathrm{d}^3\vec{r}\ \psi_j(i\hbar\vec{\nabla}\psi_i^*) &= i\hbar\int \mathrm{d}^3\vec{r}\ \vec{\nabla}(\psi_j\psi_i^*) - \int \mathrm{d}^3\vec{r}\ \vec{\nabla}\psi_j(i\hbar\psi_i^*)\\ &= i\hbar\vec{\nabla}\int \mathrm{d}^3\vec{r}\ (\psi_j\psi_i^*) - \int \mathrm{d}^3\vec{r}\ \vec{\nabla}\psi_j(i\hbar\psi_i^*)\\ &= i\hbar\vec{\nabla}0 - \int \mathrm{d}^3\vec{r}\ \vec{\nabla}\psi_j(i\hbar\psi_i^*)\\ &= -\int \mathrm{d}^3\vec{r}\ \vec{\nabla}\psi_j(i\hbar\psi_i^*)\end{aligned}$$
    - Note that the left integral above goes to zero because of the boundary condition.
    - This is relevant to PSet 1, Q2a!

- 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* $\hat{\boldsymbol{O}}^{\boldsymbol{\dagger}}$. *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 $\langle\psi_i|\hat{O}|\psi_j\rangle := \int \mathrm{d}^3\vec{r}\ \psi_i^*\hat{O}\psi_j$.
  - Essentially, we're just representing this Hilbert-space integral inner product in typical inner product notation!
- 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

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

- 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

$$\hat{O}\psi_n = O_n \psi_n \qquad \hat{O}_1 \psi_n = O_{1,n} \psi_n \qquad \hat{O}_2 \psi'_m = O_{2,m} \psi'_m$$

  - Then we have that

$$\begin{aligned} \hat{O}_1 \psi_n &= O_{1,n} \psi_n \\ \hat{O}_2 \hat{O}_1 \psi_n &= O_{1,n} \hat{O}_2 \psi_n = O_{1,n} O_{2,n} \psi_n \end{aligned}$$

and

$$\begin{aligned} \hat{O}_2 \psi_n &= O_{2,n} \psi_n \\ \hat{O}_1 \hat{O}_2 \psi_n &= O_{2,n} \hat{O}_1 \psi_n = O_{2,n} O_{1,n} \psi_n \end{aligned}$$

  - 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.
$$\langle\psi|\hat{A}|\psi'\rangle = \left\langle\psi\middle|\hat{A}\psi'\right\rangle = \left\langle\hat{A}\psi\middle|\psi'\right\rangle \qquad \langle\psi|\hat{A}^2|\psi'\rangle = \left\langle\hat{A}\psi\middle|\hat{A}\psi'\right\rangle$$
  - 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* $\boldsymbol{[\hat{O}_1,\hat{O}_2]}$. *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* $\boldsymbol{\{\hat{O}_1,\hat{O}_2\}}$. *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)

- PSet 1, 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.

2.4 Discussion Section

- There's not that much content to go over today, so we'll talk about some more mathematical tools like the Dirac delta function and Fourier transforms.
- **Dirac delta function**: The function defined as follows. *Denoted by* $\boldsymbol{\delta(x-x_0)}$. *Given by*

$$\delta(x-x_0)=\begin{cases}\infty & x=x_0\\ 0 & x\neq x_0\end{cases}$$

- Useful for solving the Schrödinger equation; this is a potential that we'll solve for.
- Important application:

$$\int_a^b \mathrm{d}x\,\delta(x-x_0)f(x)=\begin{cases}f(x_0) & x_0\in[a,b]\\ 0 & \text{otherwise}\end{cases}$$

- Examples.

1. $$\int_{-5}^{5}\mathrm{d}x\,\delta(x+4)(x^2-3x+4)=x^2-3x+4\Big|_{x=-4}=32$$

2.
$$\int_0^\infty \delta(x+\pi)\cos(x) = 0$$

   - Because $x_0 = -\pi \notin [0,\infty)$.

- Defining a notion of equality.
  - Let $D_1(x), D_2(x)$ be functions of the δ-function.
    - Example: $D_1(x) = \delta(x+3)\mathrm{e}^{-3x^2}$.
  - We say that $D_1(x) = D_2(x)$ if
$$\int_{-\infty}^{\infty} \mathrm{d}x\, D_1(x)f(x) = \int_{-\infty}^{\infty} \mathrm{d}x\, D_2(x)f(x)$$
    for any smooth function f.
- δ-function equalities.
  1. $x\delta(x) = 0$.
  2. $\delta(x) = \delta(-x)$.
  3. $\delta(cx) = \frac{1}{|c|}\delta(x)$.
  4. $\int_{-\infty}^{\infty} \mathrm{d}x\, \delta(a-x)\delta(x-b) = \delta(a-b)$.
  5. $g(x)\delta(x-a) = g(a)\delta(x-a)$.
- These equalities will probably come in handy when we start working with the δ-function.
- We can prove these five equalities with the notion of equality defined above.
- Example: Proving equality 1.

Proof. Let $D_1(x) = x\delta(x)$ and $D_2(x) = 0$. Then
$$\int_{-\infty}^{\infty} \mathrm{d}x\, \delta(x)xf(x) = xf(x)\bigg|_{x=0} = 0$$
and
$$\int_{-\infty}^{\infty} \mathrm{d}x\, 0f(x) = 0$$
It follows by transitivity that the two integrals equal each other, so we must have $x\delta(x) = 0$ as desired. □

- Equality 4 is the hardest to prove. We will have a constant $D_1(x)$ equal to
$$D_1(x) = \int_{-\infty}^{\infty} \mathrm{d}y\, \delta(a-y)\delta(y-b)$$
- Fourier transforms (FT) of δ-functions.
- Recall:
  - The FT of the function $\phi(x)$ is
$$\tilde{\phi}(k) := \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{d}x\, \mathrm{e}^{-ikx}\phi(x)$$

- The inverse FT is

$$\phi(x) := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}k \, \mathrm{e}^{ikx} \tilde{\phi}(k)$$

- We call the FT of $\delta(x - x_0)$ the function

$$\tilde{\phi}(k; x_0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}x \, \mathrm{e}^{-ikx} \delta(x - x_0) = \frac{1}{\sqrt{2\pi}} \mathrm{e}^{-ikx} \bigg|_{x=x_0} = \frac{1}{\sqrt{2\pi}} \mathrm{e}^{-ikx_0}$$

- In addition:

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}k \, \mathrm{e}^{ikx} \qquad\qquad \tilde{\delta}(k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}x \, \mathrm{e}^{-ikx}$$

- Matt explains the FT in terms of decomposing sums of sines and cosines.
- Now the physics starts!
- Expectation values.
- So far, we have the wavefunction $\psi(x)$, which mysteriously contains information on the particle.
  - It solves the Schrödinger equation.
- $|\psi(x)|^2$ gives the probability density of finding the particle at x.
- The expectation value of some function $f(x)$ is

$$\langle f(x) \rangle = \int_{-\infty}^{\infty} \mathrm{d}x \, \psi^*(x) f(x) \psi(x)$$

- 1D momentum $\hat{p}$ can be written as the operator $-i\hbar \, \partial/\partial x$. Thus,

$$\langle p \rangle = \int_{-\infty}^{\infty} \mathrm{d}x \, \psi^* = \int_{-\infty}^{\infty} \mathrm{d}x \, \psi^* \left(-i\hbar \frac{\partial \psi}{\partial x} \right)$$

  - This holds for n^{th} powers:

$$\langle \hat{p}^n \rangle = \int_{-\infty}^{\infty} \mathrm{d}x \, \psi^* (-i\hbar)^n \frac{\partial^n \psi}{\partial x^n}$$

- Example (PSet 1, Q2): Prove that

$$\langle f(p) \rangle = \int_{-\infty}^{\infty} \mathrm{d}k \, f(\hbar k) |\tilde{\psi}(k)|^2$$

Proof. Start from

$$\langle f(p) \rangle = \int_{-\infty}^{\infty} \mathrm{d}x \, \psi^*(x) f(p) \psi(x)$$

Taylor expand about $f(0)$:

$$\begin{aligned}
f(p) = f(0) + \frac{\partial f}{\partial p}\bigg|_{p=0} p + \frac{1}{2!} \frac{\partial^2 f}{\partial p^2}\bigg|_{p=0} p^2 + \cdots &= \sum_{n=0}^{\infty} \frac{1}{n!} \frac{\partial^n f}{\partial p_n^n}\bigg|_{p=0} \\
&= \int_{-\infty}^{\infty} \mathrm{d}x \, \psi^*(x) \sum_{n=0}^{\infty} \frac{1}{n!} \frac{\partial^n f}{\partial p^n}\bigg|_{p=0} p^n \psi(x) \\
&= \sum_{n=0}^{\infty} \frac{1}{n!} \frac{\partial^n f}{\partial p^n}\bigg|_{p=0} \int_{-\infty}^{\infty} \mathrm{d}x \, \psi^*(x) p^n \psi(x) \\
&= \sum_{n=0}^{\infty} \frac{1}{n!} \frac{\partial^n f}{\partial p^n}\bigg|_{p=0} \langle p^n \rangle
\end{aligned}$$

This holds when

$$
\begin{aligned}
\langle p^n\rangle &= \int_{-\infty}^{\infty}\mathrm{d}x\,\psi^*(x)(-i\hbar)^n\frac{\partial^n\psi}{\partial x^n}\\
&= \int_{-\infty}^{\infty}\mathrm{d}x\left(\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\mathrm{d}k\,\mathrm{e}^{ikx}\psi(x)\right)^*(-i\hbar)^n\frac{\partial^n}{\partial x^n}\left(\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\mathrm{d}\ell\,\mathrm{e}^{i\ell x}\tilde{\psi}(\ell)\right)\\
&= \frac{(-i\hbar)^n}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}x\int_{-\infty}^{\infty}\mathrm{d}k\int_{-\infty}^{\infty}\mathrm{d}\ell\,\mathrm{e}^{-ikx}\tilde{\psi}^*(k)\tilde{\psi}(\ell)\frac{\partial^n}{\partial x^n}(\mathrm{e}^{i\ell x})\\
&= \frac{(-i\hbar)^n}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}x\,\mathrm{d}k\,\mathrm{d}\ell\,\mathrm{e}^{-ikx}\tilde{\psi}^*(k)\tilde{\psi}(\ell)(i\ell)^n\mathrm{e}^{i\ell x}\\
&= \int_{-\infty}^{\infty}\mathrm{d}k\int_{-\infty}^{\infty}\mathrm{d}\ell\,\tilde{\psi}^*(k)\tilde{\psi}(\ell)(\ell\hbar)^n\underbrace{\frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}x\,\mathrm{e}^{i(\ell-k)x}}_{\tilde{\delta}(\ell-k)}\\
&= \int_{-\infty}^{\infty}\mathrm{d}k\,\tilde{\psi}^*(k)\tilde{\psi}(\ell)(\ell\hbar)^n\bigg|_{\ell=k}\\
&= \int_{-\infty}^{\infty}\mathrm{d}k\,\tilde{\psi}^*(k)\tilde{\psi}(k)(k\hbar)^n\\
&= \sum_{n=0}^{\infty}\frac{1}{n!}\,\frac{\partial^n f}{\partial p^n}\bigg|_{p=0}\int_{-\infty}^{\infty}\mathrm{d}k\,(k\hbar)^n|\tilde{\psi}(k)|^2\\
&= \int_{-\infty}^{\infty}\mathrm{d}k\,|\tilde{\psi}(k)|^2\underbrace{\sum_{n=0}^{\infty}\frac{1}{n!}\,\frac{\partial^n f}{\partial p^n}\bigg|_{p=0}(k\hbar)^n}_{f(k\hbar)}\\
&= \int_{-\infty}^{\infty}\mathrm{d}k\,|\tilde{\psi}(k)|^2 f(k\hbar)
\end{aligned}
$$

□

- This example is much more complicated than the PSet. If we can understand 50% of it, we'll be great. If we didn't understand any of it, no worries.
- It sounds like we're not required to come to discussion session this quarter either.

2.5 Simple Cases of Time-Independent Potentials

1/12:

- Super snowy day, his wife told him only 5 students will show up, he takes a pic of the filled lecture hall with a kid at the front holding up a sign that says "We are more than 5," lol!!
- Review of equations.
  - The operators $\hat{H},\hat{\vec{p}},\hat{\vec{r}},\hat{V}$.
  - The commutator $[p_i,r_j]=-i\hbar\delta_{ij}$.
  - The relation between $\langle\hat{\vec{r}}\rangle$ and $\langle\hat{\vec{p}}\rangle$, and Ehrenfest's theorem.
  - The Schrödinger equation.
  - The following equality from last time

$$
\left\langle\psi\middle|\hat{O}\psi\right\rangle=\left\langle\hat{O}^\dagger\psi\middle|\psi\right\rangle=\langle\psi|\hat{O}|\psi\rangle=\int\mathrm{d}^3\vec{r}\;\psi^*\hat{O}\psi
$$

  - A Hermitian operator is one for which $\hat{O}^\dagger=\hat{O}$.

    - These have real mean values and observables.

- **Incompatible** (operators): Two operators $\hat{O}_1, \hat{O}_2$ for which the following condition is met. *Constraint*

$$[\hat{O}_1, \hat{O}_2] \neq 0$$

  - Means that you can't simultaneously determine the values of the observables associated with $\hat{O}_1, \hat{O}_2$ with infinite precision.
  - Mathematically, this means that

$$\sigma_{\hat{O}_1}\sigma_{\hat{O}_2} \geq \frac{1}{2}\left|\langle\psi|[\hat{O}_1, \hat{O}_2]|\psi\rangle\right|$$

- We now start discussing time-independent potentials.
- What is important about these in classical mechanics?
  - Energy is conserved.
  - Classically, we demonstrated this by taking the equation

$$\begin{aligned}
\vec{v} \cdot \frac{\mathrm{d}}{\mathrm{d}t}\left(m\frac{\mathrm{d}\vec{r}}{\mathrm{d}t}\right) &= -\vec{\nabla}V(\vec{r}) \cdot \frac{\mathrm{d}\vec{r}}{\mathrm{d}t} \\
\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{m\vec{v}^{\,2}}{2}\right) &= -\frac{\mathrm{d}}{\mathrm{d}t}(V(\vec{r})) \\
\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{m\vec{v}^{\,2}}{2} + V(\vec{r})\right) &= 0 \\
\frac{\mathrm{d}E}{\mathrm{d}t} &= 0
\end{aligned}$$

- The equivalent expression in quantum mechanics is that

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(\langle\psi|\hat{H}|\psi\rangle\Big) = 0$$

  - We now prove this expression.
  - Start by considering the time variation of a generic Hermitian operator $\hat{O}$, i.e., we want

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\int \mathrm{d}^3\vec{r}\ \psi^*\hat{O}\psi\right) = \frac{\mathrm{d}}{\mathrm{d}t}\Big(\langle\psi|\hat{O}|\psi\rangle\Big)$$

  - Essentially, we have

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\Big(\langle\psi|\hat{O}|\psi\rangle\Big) &= \int \mathrm{d}^3\vec{r}\ \frac{\partial\psi^*}{\partial t}\hat{O}\psi + \int \mathrm{d}^3\vec{r}\ \psi^*\frac{\partial\hat{O}}{\partial t}\psi + \int \mathrm{d}^3\vec{r}\ \psi^*\hat{O}\frac{\partial\psi}{\partial t} \\
&= \int \mathrm{d}^3\vec{r}\ \psi^*\hat{O}\frac{\partial\psi}{\partial t} + \langle\psi|\frac{\partial\hat{O}}{\partial t}|\psi\rangle + \int \mathrm{d}^3\vec{r}\ \left(\hat{O}\frac{\partial\psi}{\partial t}\right)^*\psi \\
&= \int \mathrm{d}^3\vec{r}\ \left[\hat{O}\left(-\frac{i}{\hbar}\hat{H}\psi\right)\right]^*\psi + \int \mathrm{d}^3\vec{r}\ \psi^*\left(-\frac{i}{\hbar}\hat{O}\hat{H}\psi\right) + \left\langle\psi\middle|\frac{\partial\hat{O}}{\partial t}\middle|\psi\right\rangle \\
&= \frac{i}{\hbar}\int \mathrm{d}^3\vec{r}\ \psi^*(\hat{H}\hat{O} - \hat{O}\hat{H})\psi + \left\langle\psi\middle|\frac{\partial\hat{O}}{\partial t}\middle|\psi\right\rangle \\
\frac{\mathrm{d}}{\mathrm{d}t}\Big(\langle\psi|\hat{O}|\psi\rangle\Big) &= \frac{i}{\hbar}\langle\psi|[\hat{H}, \hat{O}]|\psi\rangle + \left\langle\psi\middle|\frac{\partial\hat{O}}{\partial t}\middle|\psi\right\rangle
\end{aligned}$$

    - In the first step, we move the derivative into the integral and do a tripartite product rule.

- The last statement above is a general statement that applies to all Hermitian operators $\hat{O}$, that is, all observables.

– Now, we can simply plug in $\hat{O} = \hat{H}$. Since the commutator of the Hamiltonian with itself is zero and $\partial\hat{H} \big/ \partial t = 0$ by hypothesis (for a time-independent potential), we have that $\mathrm{d}/\mathrm{d}t\,(\langle\psi|\hat{H}|\psi\rangle) = 0$, as desired.

- Wagner reproves that $[\hat{\vec{p}}_x, \hat{\vec{x}}] = -i\hbar$.
  - Analogously, he proves that $[\hat{\vec{p}}_x, \hat{\vec{y}}] = 0$.
  - Relevant to PSet 1, Q3b!
- Implication: You *can* have an operator with a perfectly defined x-momentum and y-position.
- Another new derivation:

$$\begin{aligned}
[\hat{\vec{p}}_x, \hat{V}(\vec{r})]f &= -i\hbar\frac{\partial}{\partial x}(V(\vec{r})f) + i\hbar V(\vec{r})\frac{\partial f}{\partial x} \\
&= -i\hbar\frac{\partial V}{\partial x}f
\end{aligned}$$

- What if we want to figure out $[\hat{\vec{p}}, \hat{V}(\vec{r})]$?
  - Start off with the expression we derived above.

$$\frac{\partial}{\partial t}\Big(\langle\psi|\hat{\vec{p}}|\psi\rangle\Big) = \frac{i}{\hbar}\langle\psi|[\hat{H},\hat{\vec{p}}]|\psi\rangle = \frac{i}{\hbar}(i\hbar\langle\psi|\vec{\nabla}V|\psi\rangle) = -\langle\psi|\vec{\nabla}V|\psi\rangle$$

- Moving on, let's try solving the Schrödinger equation with a separable ansatz,

$$\psi(\vec{r},t) = \psi(\vec{r})\phi(t)$$

  - This works because the left side of the Schrödinger equation doesn't operate on the position, and the right side doesn't operate on the time.
  - Let's begin.

$$\begin{aligned}
-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi(\vec{r},t) + V(\vec{r})\psi(\vec{r},t) &= i\hbar\frac{\partial}{\partial t}(\psi(\vec{r},t)) \\
\phi(t)\left[-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi(\vec{r}) + V(\vec{r})\psi(\vec{r})\right] &= i\hbar\psi(\vec{r})\frac{\partial}{\partial t}(\phi(t)) \\
\frac{1}{\psi(\vec{r})}\left[-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi(\vec{r}) + V(\vec{r})\psi(\vec{r})\right] &= \frac{i\hbar}{\phi(t)}\frac{\partial}{\partial t}(\phi(t))
\end{aligned}$$

  - Now the two sides of the above equation are functions of different variables, so they cannot be equal *unless* they are equal to a constant, which we'll call E. This allows us to split the above equation into two:

$$\frac{1}{\psi(\vec{r})}\hat{H}\psi(\vec{r}) = E \qquad\qquad \frac{i\hbar}{\phi(t)}\frac{\partial}{\partial t}(\phi(t)) = E$$

$$\hat{H}\psi(\vec{r}) = E\psi(\vec{r}) \qquad\qquad \phi(t) = A\exp\left(-\frac{iEt}{\hbar}\right)$$

    - A is a constant of integration.
  - We also have that

$$E_n = \langle\psi_n|\hat{H}|\psi_n\rangle$$

    - This means that the eigenstates of $\hat{H}$ correspond to eigenvalues E_n.

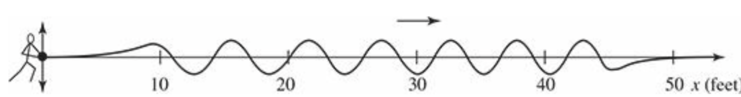
- Thus, we have
$$\psi_n(\vec{r},t) = \psi_n(\vec{r})\exp\left(-\frac{iE_nt}{\hbar}\right)$$
  - Note that we assume that we have renormalized every ψ_n written this way from here on out, absorbing A and anything with it into $\psi_n(\vec{r})$.
- When $m \neq n$, we can obtain an important rule:
$$\begin{gathered}\langle\psi_m|\hat{H}|\psi_n\rangle = E_n\langle\psi_m|\psi_n\rangle = E_m\langle\psi_m|\psi_n\rangle\\ (E_n - E_m)\langle\psi_m|\psi_n\rangle = 0\end{gathered}$$
  - It follows that if $E_m \neq E_n$, then $\langle\psi_m|\psi_n\rangle = 0$!
- Now let
$$\psi = \sum_n c_n\psi_n(\vec{r})\exp\left(-\frac{iE_nt}{\hbar}\right)$$
  - Then
$$\begin{aligned}\langle\psi|\psi\rangle &= \sum_{m,n} c_m^*c_n\exp\left(-\frac{i}{\hbar}(E_m - E_n)t\right)\langle\psi_m|\psi_n\rangle\\ &= \sum_m |c_m|^2\end{aligned}$$
  - This follows from the fact that $\langle\psi_m|\psi_n\rangle = 1$.
- Last note.
$$\begin{aligned}\langle\psi|\hat{H}|\psi\rangle &= \sum_{m,n} c_m^*c_n\exp\left(-\frac{i}{\hbar}(E_m - E_n)t\right)\underbrace{\langle\psi_m'|\hat{H}|\psi_n\rangle}_{E_n\langle\psi_m|\psi_n\rangle}\\ &= \sum_m |c_m|^2E_m\end{aligned}$$

2.6 Chapter 1: The Wave Function

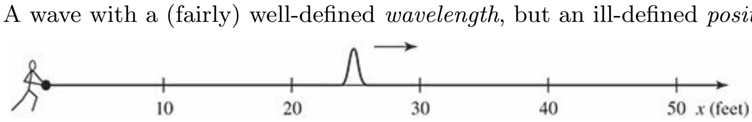
From Griffiths and Schroeter (2018).

Section 1.6: The Uncertainty Principle

1/29: - Qualitative justification of the uncertainty principle.



(a) A wave with a (fairly) well-defined *wavelength*, but an ill-defined *position*.



(b) A wave with a (fairly) well-defined *position*, but an ill-defined *wavelength*.

Figure 2.1: Visualizing the uncertainty principle.

  - Consider someone shaking a rope.

        - If they do so a lot, you get a wave with a well-defined wavelength and ill-defined position.
        - If they just shake it once, you get a wave with a well-defined position and ill-defined wavelength.
    - Thus, we see that there is a tradeoff between measuring the precision of wavelength and position.
    - This discussion is adapted from a quantitative theorem of Fourier analysis that is beyond the scope of the book.

- For a wave function, recall that de Brogelie said $\lambda \propto 1/p$, so the above relation between the uncertainties in position and wavelength becomes — for a quantum particle — a relation between the uncertainties in position and momentum.

- The Heisenberg Uncertainty Principle is stated, but not proven until Chapter 3.

2.7 Chapter 2: Time-Independent Schrödinger Equation

From Griffiths and Schroeter (2018).

Section 2.1: Stationary States

- Goes through solving the TDSE via separation of variables.
    - Remark: Separation of variables is "the physicist's first line of attack on any partial differential equation" (Griffiths & Schroeter, 2018, p. 43).
    - Griffiths and Schroeter (2018) finally addresses my criticism that separation of variables will restrict us to a tiny subset of solutions!
        - Answer: This is true, but it just so happens that the solutions we *do* get turn out to be of great interest. So essentially, this is "because it works" physics.

- **Time-independent Schrödinger equation**: The equation defined as follows. *Also known as* **TISE**. *Given by*

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}+V\psi=E\psi$$

- The remaining sections of this chapter will focus on solving the TISE for various simple potentials.

- Three reasons why separable solutions are valuable.
    1. They are **stationary states**.
        - Every expectation value $\langle Q(x,p)\rangle$ is also constant in time.
        - In particular, $\langle\hat{\vec{x}}\rangle$ is constant so $\langle\hat{\vec{p}}\rangle=0$.
    2. They are states of definite total energy.
        - Reproves that $\sigma_H^2=0$, and hence every measurement of the total energy is certain to return the value E.
    3. The general solution is a linear combination of separable solutions.
        - Essentially, we can prove that *every* solution to the TDSE can be written as

$$\psi(x,t)=\sum_{n=0}^{\infty}c_n\psi_n(x)\mathrm{e}^{-iE_nt/\hbar}$$

- **Stationary state**: A wave function $\psi(x,t)$ for which the probability density $|\psi(x,t)|^2$ does *not* depend on t.

- Example: The linear combination of two stationary states produces motion.

  - If $\psi(x,0) = c_1\psi_1(x) + c_2\psi_2(x)$, then we may compute that

$$|\psi(x,t)|^2 = c_1^2\psi_1^2 + c_2^2\psi_2^2 + 2c_1c_2\psi_1\psi_2\cos\left(\frac{E_2 - E_1}{\hbar}t\right)$$

- $|c_n|^2$ is the probability that a measurement of the energy would return the value E_n.
  - Proven in Chapter 3.
- It follows from this understanding that we must have Wagner's favorite two equations,

$$\sum_{n=0}^{\infty}|c_n|^2 = 1 \qquad\qquad \sum_{n=0}^{\infty}|c_n|^2 E_n = \langle\hat{H}\rangle$$

- Remark: "Because the constants $\{c_n\}$ are independent of time, so too is the probability of getting a particular energy, and, *a fortiori*, the expectation value of H. These are manifestations of energy conservation in quantum mechanics" (Griffiths & Schroeter, 2018, p. 47).

Week 3

Time-Independent Problems in One-Dimensional Systems

3.1 Infinite Well Motion

1/17:

- We begin today by building up to the uncertainty principle another, more general way.
- Recall that what we are aiming for is

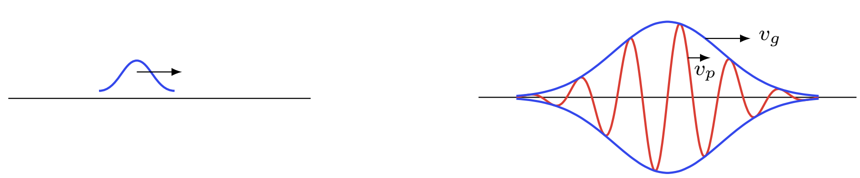
$$\Delta p_x \Delta x \geq \frac{\hbar}{2}$$

  where $\Delta p_x, \Delta x$ are the uncertainties in the determination of the momentum and position, respectively:

$$(\Delta p_x)^2 = \langle(\hat{\vec{p}}_x - \langle\hat{\vec{p}}_x\rangle)^2\rangle = \langle\hat{\vec{p}}_x{}^2\rangle - \langle\hat{\vec{p}}_x\rangle^2 \qquad (\Delta x)^2 = \langle\hat{\vec{x}}^2\rangle - \langle\hat{\vec{x}}\rangle^2$$

- Example of the uncertainty principle: For a plane wave, we know the momentum but not the position. That is, $\Delta x \to \infty$ and $\Delta p_x \to 0$.
- More generally, for a **wave packet**, we know only approximately the position and momentum.
- **Wave packet**: A continuous sum of waves of different frequencies. *Given by*

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) \mathrm{e}^{i(kx - \omega(k)t)} \,\mathrm{d}k$$



(a) A wave packet. (b) Group and phase velocity.

Figure 3.1: Wave packets.

  - Note that the above formula only applies to the one dimensional case.
- Let's investigate the case of a wave packet of free particles.
  - In this case,

$$\omega(k) = \frac{\hbar k^2}{2m}$$

    - This is derived from
      $$\hbar\omega = E = \frac{p^2}{2m} = \frac{(\hbar k)^2}{2m}$$
      by cancelling an $\hbar$ from both sides.
  - Let's assume that $\phi(k)$ is a narrowly peaked function around a certain value k_0.
  - Then we can expand
    $$\begin{aligned}\omega(k) &= \omega(k_0) + \left.\frac{\mathrm{d}\omega}{\mathrm{d}k}\right|_{k=k_0}(k-k_0)+\cdots\\ &= \omega(k_0) + \left.\frac{\hbar k}{m}\right|_{k=k_0}(k-k_0)+\cdots\\ &= \omega(k_0) + \underbrace{\frac{\hbar k_0}{m}}_{\omega_0'}(k-k_0)+\cdots\end{aligned}$$
  - Define $s := k - k_0$.
  - Then $k = k_0 + s$ and $\mathrm{d}k = \mathrm{d}s$, so
    $$\begin{aligned}\psi(x,t) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\phi(k_0+s)\mathrm{e}^{i((k_0+s)x-(\omega(k_0)+\omega_0' s)t)}\,\mathrm{d}s\\ &= \frac{1}{\sqrt{2\pi}}\mathrm{e}^{i(k_0x-\omega(k_0)t)}\int_{-\infty}^{\infty}\phi(k_0+s)\mathrm{e}^{is(x-\omega_0't)}\,\mathrm{d}s\end{aligned}$$
  - It follows that
    $$|\psi(x,t)|^2 = \frac{1}{2\pi}\left|\int_{-\infty}^{\infty}\phi(k_0+s)\mathrm{e}^{is(x-\omega_0't)}\,\mathrm{d}s\right|^2 = f(x-\omega_0't)$$
    - In words, the probability density is a function of $x-\omega_0't$, so the packet moves with **group velocity** $\omega_0' = \hbar k_0/m = p_0/m$.
  - Implication: The wave packet moves with a velocity that is equal ot the classical velocity
    $$\left.\frac{\mathrm{d}\omega}{\mathrm{d}k}\right|_{k=k_0} = \frac{p_0}{m}$$
- **Group velocity**: A measure of the velocity of a wave packet. *Denoted by* $\boldsymbol{v_g}$, $\boldsymbol{v_{\text{group}}}$. *Given by*
  $$v_{\text{group}} = \left.\frac{\mathrm{d}\omega}{\mathrm{d}k}\right|_{k=k_0}$$
- **Phase velocity**: A measure of the velocity of the ripples. *Denoted by* $\boldsymbol{v_p}$, $\boldsymbol{v_{\text{phase}}}$. *Given by*
  $$v_{\text{phase}} = \frac{\omega(k_0)}{k_0} = \frac{\hbar k_0}{2m} = \frac{v_{\text{group}}}{2}$$
- Explicit example of a wave packet: A **Gaussian wave packet**.
- **Gaussian wave packet**: A one-dimensional wave packet of the following form. *Given by*
  $$\psi_0(x,t) = \left(\frac{2}{\pi\sigma^2}\right)^{1/4}\exp\left[-\frac{(x-v_gt)^2}{\sigma^2}\right]\mathrm{e}^{i(k_0x-v_pt)}$$
  - This means that we must have used the following definition of $\phi(k)$ in the original definition.
    $$\phi(k) = \left(\frac{\sigma^2}{2\pi}\right)^{1/4}\exp\left[-\frac{\sigma^2(k-k_0)^2}{4}\right]$$

- Uncertainty analysis of a Gaussian wave packet.
  - The uncertainties Δx and Δk are associated with the widths of the Gaussians, as one can determine by computing. Indeed, at $t = 0$,

$$\langle \hat{\vec{x}} \rangle = 0 \qquad \langle \hat{\vec{x}}^{\,2} \rangle = (\Delta x)^2 \qquad \langle (k - k_0)^2 \rangle = (\Delta k)^2$$

    - Indeed, since $\langle k \rangle = k_0$, we know that $\langle (k-k_0)^2 \rangle = \langle k^2 \rangle - k_0^2$.
  - For Gaussians, normalized as $\int |\psi|^2 = 1$, we obtain

$$\left(\frac{1}{\pi \sigma^2} \right)^{1/2} \int_{-\infty}^{\infty} u^2 \exp\left(-\frac{u^2}{\sigma^2} \right) \mathrm{d}u = (\Delta u)^2 = \frac{\sigma^2}{2}$$

    - How do we get this??
  - It follows that the value of Δu coincides well with the departure from the central value for which the exponential in $|\psi|^2$ or $|\phi|^2$ is $\mathrm{e}^{-1/2}$.
  - Altogether, we get

$$\Delta x = \frac{\sigma}{2} \qquad \Delta k = \frac{1}{\sigma}$$

    so

$$\begin{aligned} \Delta x \Delta k &= \frac{1}{2} \\ \Delta x \Delta p_x &= \frac{\hbar}{2} \end{aligned}$$

    for a Gaussian wave packet.
  - Implication: The Gaussian function minimizes the product of the position and momentum uncertainties!
- We now move onto discussing the **infinite square well** potential, a one-dimensional time-independent potential for which we can solve the Schrödinger equation exactly.

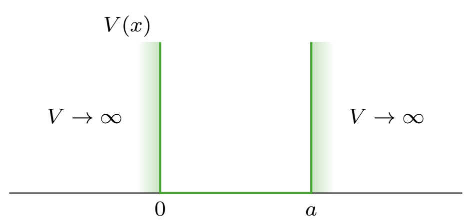


Figure 3.2: Infinite square well.

- **Infinite square well**: The potential energy function that vanishes for $0 < x < a$ and tends to infinity for $x \leq 0$ and $x \geq a$. *Given by*

$$V(x) = \begin{cases} 0 & 0 < x < a \\ \infty & \text{otherwise} \end{cases}$$

- We would like to obtain energy eigenstates for this potential. That is, we seek eigenvalues and eigenfunctions for

$$\left[-\frac{\hbar^2}{2m} \frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x) \right] \psi(x) = E\psi(x)$$

  - Any such eigenstate ψ will have $\psi(x) = 0$ in the region of space where $V \to \infty$.

- Hence, the Schrödinger equation reduces to the boundary-value problem

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = E\psi \qquad\qquad \psi(0) = \psi(a) = 0$$

- The above ODE may be expressed in the following equivalent form

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = -\left(\frac{2mE}{\hbar^2}\right)\psi$$

- Observe that this ODE is of the same form as the classical harmonic oscillator equation $\mathrm{d}^2x/\mathrm{d}t^2 = -(k/m)x$. Thus, it admits a similar set of solutions:

$$\psi_n(x) = C\sin\left(\sqrt{\frac{2mE_n}{\hbar^2}}x\right) \qquad\qquad \sqrt{\frac{2mE_n}{\hbar^2}}a = n\pi,\ n = 1, 2, \dots$$

- It follows that

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2}$$

- The coefficient C can be fixed via the normalization requirement, as follows.

$$\begin{aligned}
1 &= \int_0^a |\psi_n(x)|^2 \,\mathrm{d}x \\
&= C^2 \int_0^a \sin^2\left(\frac{\pi n x}{a}\right)\mathrm{d}x \\
&= C^2 \int_0^a \frac{1-\cos\left(\frac{2\pi n x}{a}\right)}{2}\,\mathrm{d}x \\
&= \frac{C^2}{2}\left[\int_0^a \mathrm{d}x - \int_0^a \cos\left(\frac{2\pi n x}{a}\right)\mathrm{d}x\right] \\
&= \frac{C^2}{2}\left[a - \underbrace{\frac{a}{2n\pi}\sin\left(\frac{2\pi n x}{a}\right)\Big|_0^a}_{0}\right] \\
&= \frac{aC^2}{2} \\
C &= \sqrt{\frac{2}{a}}
\end{aligned}$$

- Therefore, the complete eigenfunctions and eigenvalues are

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi n x}{a}\right) \qquad\qquad E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2}$$

- A general solution is therefore given by the following, where ψ_n, E_n are defined as above.

$$\psi(x,t) = \sum_n c_n \psi_n(x)\mathrm{e}^{-iE_n t/\hbar}$$

- The probability density of the infinite square well potential is time-independent.

  Proof. Observe that given any individual eigenstate of energy

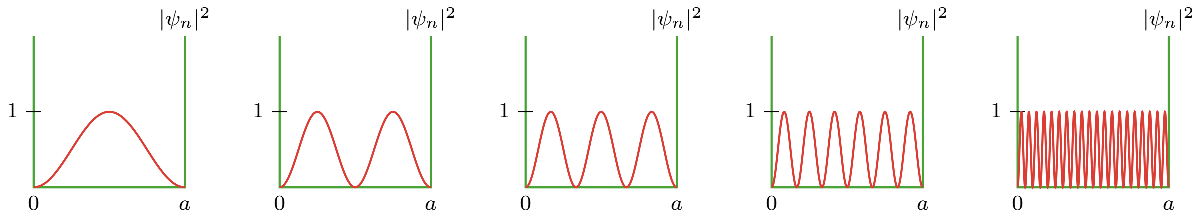
$$\psi_n(x,t) = \psi_n(x)\mathrm{e}^{-iE_n t/\hbar}$$

  we have that

$$|\psi_n(x,t)|^2 = |\psi_n(x)|^2 = \frac{2}{a}\sin^2\left(\frac{\pi n x}{a}\right)$$

$\square$

- Let's investigate the form of the probability density for a few n.

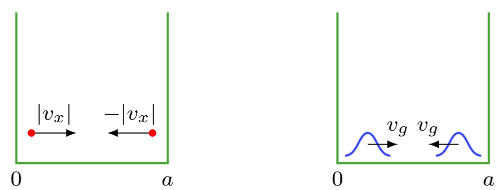


(a) $n = 1$. (b) $n = 2$. (c) $n = 3$. (d) $n = 6$. (e) $n \gg 1$.

Figure 3.3: Infinite square well probability density.

  - Recall that the average height of a sine wave is half its amplitude. Thus the average probability density is
$$\frac{1}{2} \cdot \frac{2}{a} = \frac{1}{a}$$

- Recovering "motion," in the sense that $\mathrm{d}/\mathrm{d}t \left(\langle \psi | \hat{\vec{x}} | \psi \rangle \right) \neq 0$



(a) Classical. (b) Quantum.

Figure 3.4: Infinite square well motion.

  - We obtain motion upon superimposing different eigenstate wave functions.
  - Guiding question: What would happen in the classical case of a particle in such a potential?
    - The particle would move first to the right with momentum $|p_x|$, then bounce against the wall at $x = a$ and change its momentum to $-|p_x|$, then bounce against the wall at $x = 0$ and change its momentum back to $|p_x|$, and so continue indefinitely.
  - In quantum mechanics, we can mimic the same behavior by forming a wave packet!
  - Since the particle moves free of forces between $0 < x < a$, one can try to build a Gaussian wave packet, similar to the one we discussed in the free particle case. The difference is that any wave function must vanish at $x = 0, a$, so it must be represented not by combinations of free waves e^{ikx} at $t = 0$ but by
$$\sin\left(\frac{\pi n x}{a}\right) = \frac{1}{2i}(\mathrm{e}^{i\pi n x/a} - \mathrm{e}^{-i\pi n x/a})$$
  - Define
$$k_n = \frac{\sqrt{2mE_n}}{\hbar} = \frac{\pi n}{a}$$
  - Now, what we want is a Gaussian with width Δx for $\Delta x \ll a$.
  - Recalling the free case $|\psi_0(x,t)|^2 = (1/\pi\sigma^2)^{1/2}\mathrm{e}^{-(x-v_g t)^2/2\sigma^2}$ with $\phi(k) = k\mathrm{e}^{-\sigma^2(k-k_0)^2}$, we would like to try
$$\phi(k_n) \propto \mathrm{e}^{-\sigma^2(k_n-k_0)^2} =: c_n$$
where $\sigma = \Delta x \ll a$, and hence $1/\sigma \gg 1/a$.

- Since
$$k_m - k_n = (m-n)\frac{\pi}{a}$$
we will obtain a "continuous" distribution of states with $|k_n - k_0| < 1/\sigma$ as well as a suppression of other modes.
- Left as an exercise to the student to derive further results about this system.

3.2 Harmonic Oscillator

1/19:

- The harmonic oscillator is one of the most important problems in physics because we can solve it exactly.
- It used to approximate solutions near the bottom of smooth potential wells. It does so via
$$V(x) \approx V(x_0) + \left.\frac{\mathrm{d}V}{\mathrm{d}x}\right|_{x_0}(x-x_0) + \frac{1}{2}\left.\frac{\mathrm{d}^2V}{\mathrm{d}x^2}\right|_{x_0}(x-x_0)^2 + \cdots$$
  - Mathematically, this represents small departures from x_0.
  - Recall that the first derivative goes to zero (because we are at a minimum) and the second one is a constant we can call k, yielding
$$V(x) = V(x_0) + \frac{1}{2}k(x-x_0)^2$$
  - This is now a potential with which we are familiar from classical mechanics.
- Recall what happens in classical mechanics.
  - We get an equation with a second derivative of $u = x - x_0$:
$$m\frac{\mathrm{d}^2u}{\mathrm{d}t^2} = -ku$$
  - This problem is solved in classical mechanics by defining $\omega^2 := k/m$ and solving the differential equation for
$$u = A\sin(\omega t) + B\cos(\omega t)$$
  - From this general solution, we can get to particular solutions using initial conditions.
  - For example, if $u(0) = 0$, then $B = 0$ and
$$u = A\sin(\omega t)$$
  - What happens if we multiply the original equation of motion by $v = \mathrm{d}u/\mathrm{d}t$? We get the conservation of energy!
$$mv\frac{\mathrm{d}v}{\mathrm{d}t} = -ku\frac{\mathrm{d}u}{\mathrm{d}t}$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{mv^2}{2} + \frac{ku^2}{2}\right) = 0$$
  - Note that we associate the left term above with $KE = p^2/2m$ and the right term above with $V(u)$.

- This gives us

$$V(u) = \frac{ku^2}{2} = \frac{k[A\sin(\omega t)]^2}{2} = \frac{kA^2}{2}\sin^2(\omega t)$$
$$K(u) = \frac{mv^2}{2} = \frac{m}{2}\left(\frac{\mathrm{d}}{\mathrm{d}t}[A\sin(\omega t)]\right)^2 = \frac{A^2 m\omega^2}{2}\cos^2(\omega t) = \frac{kA^2}{2}\cos^2(\omega t)$$

so that

$$V(u) + K(u) = \frac{kA^2}{2}$$

for all u!

- The situation is different in quantum mechanics.
  - Here, we must begin from

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi_n(x) + \frac{kx^2}{2}\psi_n(x) = E_n\psi_n(x)$$

- What do we know, qualitatively, about a solution to this ODE?
  - Since $V(x)$ is time-independent, the eigenfunctions will be of the form

$$\psi_n(x,t) = \psi_n(x)\mathrm{e}^{-iE_n t/\hbar}$$

  - We will be able to normalize these solutions via

$$\int \mathrm{d}x\, \psi_m^*(x)\psi_n(x) = \delta_{nm}$$

  - The general solution will then be a sum of the normalized solutions, like the following.

$$\psi(x,t) = \sum_n c_n\psi_n(x,t)$$

  - The normalization condition *here* will then yield

$$\sum_n |c_n|^2 = 1$$

  - Lastly, we will be able to calculate expected values, such as

$$\langle\psi|\hat{H}|\psi\rangle = \sum_m |c_m|^2 E_m$$

- We now work toward quantitative solutions $\psi_n(x,t)$, based on insight from the following picture.

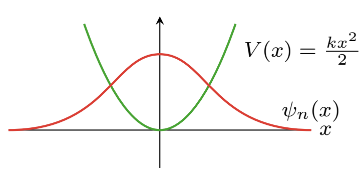


Figure 3.5: Solving the quantum harmonic oscillator with an asymptotic Schrödinger equation.

  - Although it may not be immediately obvious how to solve the Schrödinger equation in this case, we can see from Figure 3.5 that at large values of x, $\psi_n(x) = 0$. Thus, for large x, we will have

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi_n(x) + \frac{kx^2}{2}\psi_n(x) = 0$$

    - This tells us the **asymptotic** behavior of the equation.

  - We can then algebraically rearrange this equation into the form

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi_n(x) - \frac{m^2\omega^2x^2}{\hbar^2}\psi_n(x) = 0$$

  - To solve it, use an ansatz proportional to the following.

$$\psi_n(x) \propto \exp\Big[-\frac{m\omega}{2\hbar}x^2\Big]$$

    - This works because

$$\begin{aligned}\frac{\mathrm{d}\psi_n}{\mathrm{d}x} &= -\frac{m\omega x}{\hbar}\exp\Big[-\frac{m\omega}{2\hbar}x^2\Big]\\ \frac{\mathrm{d}^2\psi_n}{\mathrm{d}x^2} &= \left(-\frac{m\omega}{\hbar} + \frac{m^2\omega^2x^2}{\hbar^2}\right)\exp\Big[-\frac{m\omega}{2\hbar}x^2\Big]\end{aligned}$$

  - In particular, use the ansatz

$$\psi_n(x) = f_n(x)\exp\Big[-\frac{m\omega}{2\hbar}x^2\Big]$$

  - Now insert this ansatz into the original equation and solve for values of $f_n(x)$ that give an exact solution.
  - Start by calculating that

$$\frac{\mathrm{d}\psi_n}{\mathrm{d}x} = \frac{\mathrm{d}f_n(x)}{\mathrm{d}x}\exp\Big[-\frac{m\omega}{2\hbar}x^2\Big] - f_n(x)\frac{m\omega x}{\hbar}\exp\Big[-\frac{m\omega}{2\hbar}x^2\Big]$$

  and thus

$$\begin{aligned}\frac{\mathrm{d}^2\psi_n}{\mathrm{d}x^2} &= \frac{\mathrm{d}^2f_n(x)}{\mathrm{d}x^2}\exp\Big[-\frac{m\omega}{2\hbar}x^2\Big] - 2\frac{\mathrm{d}f_n(x)}{\mathrm{d}x}\frac{m\omega x}{\hbar}\exp\Big[-\frac{m\omega}{2\hbar}x^2\Big]\\ &\quad - f_n(x)\frac{m\omega}{\hbar}\exp\Big[-\frac{m\omega}{2\hbar}x^2\Big] + f_n(x)\frac{m^2\omega^2x^2}{\hbar^2}\exp\Big[-\frac{m\omega}{2\hbar}x^2\Big]\\ &= \left[f_n''(x) - \frac{2m\omega x}{\hbar}f_n'(x) - f_n(x)\frac{m\omega}{\hbar} + f_n(x)\frac{m^2\omega^2x^2}{\hbar^2}\right]\exp\Big[-\frac{m\omega}{2\hbar}x^2\Big]\\ &= \left[f_n''(x) - \frac{2m\omega x}{\hbar}f_n'(x) + \frac{m\omega}{\hbar}\left(\frac{m\omega x^2}{\hbar} - 1\right)f_n(x)\right]\exp\Big[-\frac{m\omega}{2\hbar}x^2\Big]\end{aligned}$$

  - Now we insert the above into the full original Schrödinger equation, cancelling the exponential term immediately to save space.

$$\begin{aligned}-\frac{\hbar^2}{2m}\left[f_n''(x) - \frac{2m\omega x}{\hbar}f_n'(x) + \frac{m\omega}{\hbar}\left(\frac{m\omega x^2}{\hbar} - 1\right)f_n(x)\right] + \frac{m\omega^2x^2}{2}f_n(x) &= E_nf_n(x)\\ -\frac{\hbar^2}{2m}\left(f_n'' - \frac{2m\omega x}{\hbar}f_n' - \frac{m\omega}{\hbar}f_n\right) &= E_nf_n\\ -\frac{\hbar^2}{2m}f_n'' + \hbar\omega xf_n' + \left(\frac{\hbar\omega}{2} - E_n\right)f_n &= 0\end{aligned}$$

- Thus, we have obtained an ODE that we can solve to find particular solutions.
- One obvious solution: the **minimal energy solution**.
- **Minimal energy solution** (to the quantum harmonic oscillator): Take f_n to be a constant C. *Given by*

$$\psi_0(x) = C\exp\Big[-\frac{m\omega}{2\hbar}x^2\Big] \qquad\qquad E_0 = \frac{\hbar\omega}{2}$$

  - Note that it is the above ODE that necessitates $E_0 = \hbar\omega/2$ if f_n is to be a constant.
  - The minimal energy solution classically is zero, but in quantum mechanics, there will always be some energy!
    - Zero energy is impossible because it would imply that the position and momentum are both zero. But there needs to be some uncertainty, in both, so the position and momentum *cannot* both be zero.
    - Essentially, the uncertainty principle *necessitates* a finite nonzero minimal energy. Stated another way, zero energy is *inconsistent* with the uncertainty principle.

- What if we postulate that $f_1 = b_1 x$ for some constant b_1?
  - Then the ODE simplifies to

$$\begin{aligned}\hbar\omega b_1 x + \left(\frac{\hbar\omega}{2} - E_1\right) b_1 x &= 0\\ E_1 &= \frac{3\hbar\omega}{2}\end{aligned}$$

  - Note that

$$E_1 - E_0 = \hbar\omega$$

    - This observation is important because we can actually prove that

$$E_{n+1} - E_n = \hbar\omega$$

      for all $n = 0, 1, 2, \dots$.
    - We will not prove this in this class, though; we will just postulate it.
    - Essentially, what we do is assume that

$$f_N(x) = \sum_{n=1}^{N} b_n x^n$$

      and solve.
    - All the solutions are either even or odd solutions based on whether N is even or odd. These "even" and "odd" solutions correspond to even and odd polynomial functions.
  - This means that

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

- In particular, if we let $\xi = x\sqrt{m\omega/\hbar}$, then the solutions f_N are the **Hermite polynomials**.
- **Hermite polynomial**: A polynomial of the following form. *Denoted by* $\boldsymbol{H_n(\xi)}$. *Given by*

$$H_n(\xi) = (-1)^n \exp(\xi^2) \frac{\mathrm{d}^n}{\mathrm{d}\xi^n}[\exp(-\xi^2)]$$

- Thus, the general solutions to the quantum harmonic oscillator

$$\psi_n(x) = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \frac{H_n(\xi)}{\sqrt{2^n n!}} \exp\left[-\frac{\xi^2}{2}\right]$$

- On Monday, we will derive this result using **rasing** and **lowering** operators.

3.3 Office Hours (Wagner)

- PSet 2, Q1: Do you want us to rederive the wavefunction, or just answer the questions in the parts?
- Do we have to show our integration steps, or are integral calculators fine?
  - Show whatever we feel comfortable with.
  - Sounds like Wagner thinks we should be able to do all these calculations like we were born doing them, but integral calculators and skipping steps shouldn't lose us any points.
- Including Problem 3 was probably a mistake, but now that it's included, we have to do it.
- PSet 2, Q1d:
  - One way to do this problem is to remember that $\mathrm{d}\langle\hat{r}\rangle/\mathrm{d}t = \langle p\rangle/m$ and $\mathrm{d}\langle p\rangle/\mathrm{d}t = 0$.
  - Now the $\psi = \sum_n c_n \sin(k_n x)$.
  - The mean value of the momentum, once computed explicitly, is

$$\langle p\rangle \propto \int \mathrm{d}x \left[\sum_n c_n \sin(k_n x) \cdot \frac{\partial}{\partial x}\left(\sum_n c_n \sin(k_n x)\right)\right]$$

  - Then we integrate using the trick that

$$\sin x \cos y = \frac{1}{2}\sin(x+y) + \frac{1}{2}\sin(x-y)$$

    - Wagner briefly proves this trig identity.
  - Recall tricks like given an *even* function f,

$$\int_{-L}^{L} \mathrm{d}x\, x \cdot f(x) = 0$$

- PSet 2, Q2:
  - There is some part where we do not need to find exact solutions.

3.4 Chapter 2: Time-Independent Schrödinger Equation

From Griffiths and Schroeter (2018).

Section 2.2: The Infinite Square Well

1/29:
- Goes through the derivation from class.
- The boundary conditions will be justified in Section 2.5!
- Note that since A is complex, normalization technically only determines the magnitude $|A|$. However, the phase of A carries no physical significance, so there is no reason not to choose the simplest solution to $|A|^2 = 2/a$, which is just the positive real square root.
- Notice how, as promised, the TISE delivers a set $\{\psi_n(x)\}$ of solutions!
- **Ground state**: The wave functional solution to the TISE which carries the lowest energy.
- **Excited state**: Any wave functional solution to the TISE that is not the ground state.
- Four properties of the ψ_n of the infinite square well.

1. They are alternately even and odd, with respect to the center of the well.
2. As E_n increases, each successive state has one more **node**.
3. The $\{\psi_n\}$ are mutually orthogonal.
   - Griffiths and Schroeter (2018) proves that any ψ_n, ψ_m ($n \neq m$) are orthogonal.
4. The $\{\psi_n\}$ are **complete**.

- **Complete** (set of functions): A set of functions such that any other function $f(x)$ can be expressed as a linear combination of them.
  - Griffiths and Schroeter (2018) will not prove the completeness of the functions $\sqrt{2/a}\sin(\pi nx/a)$, but the mathematically inclined student may notice that an infinite sum of these is the **Fourier series** for $f(x)$, and the fact that any function can be expanded in this way is called **Dirichlet's theorem**.
  - To compute the c_n corresponding to an arbitrary f, use **Fourier's trick**:

$$\int \psi_m^*(x)f(x)\,\mathrm{d}x = \sum_{n=1}^{\infty} c_n \int \psi_m^*(x)\psi_n(x)\,\mathrm{d}x = \sum_{c_n} \delta_{mn} = c_m$$

  - Aside (from me): Dirac notation expresses the above statement as simply a consequence of taking the inner product of a vector and a member of the orthonormal basis.

$$\langle \psi_m | f \rangle = c_m$$

- Note on the four properties.
  - Property 1 is true whenever the potential is a symmetric function.
  - Property 2 is universal, regardless of the shape of the potential.
  - Orthogonality is quite general (we'll see exactly how much in Chapter 3).
  - Completeness holds for all potentials we are likely to encounter (but the proofs tend to be nasty).
    - "Most physicists simply *assume* completeness, and hope for the best" (Griffiths & Schroeter, 2018, p. 52).
- With what we know now, we can compute the time evolution of any particle in this system.
  - Simply start with its wave function at $t = 0$, which is $\psi(x, 0)$.
  - Compute expansion coefficients.
  - And take $\psi(x, t)$ to be the sum of stationary states.
- Griffiths and Schroeter (2018) proves — as at the end of class on 1/12 — that $\sum_n |c_n|^2 = 1$ and $\sum_n |c_n|^2 E_n = \langle H \rangle$.

Week 4

Observables and Hermitian Operators

4.1 Harmonic Oscillator: Raising and Lowering Operators

1/22:

- **Raising operator**: The operator defined as follows. *Denoted by* $\hat{\boldsymbol{a}}_+$, $\boldsymbol{a}_+$. *Given by*

$$\hat{a}_+ = \frac{1}{\sqrt{2\hbar m\omega}}[-i\hat{\vec{p}} + m\omega\hat{\vec{x}}]$$

- **Lowering operator**: The operator defined as follows. *Denoted by* $\hat{\boldsymbol{a}}_-$, $\boldsymbol{a}_-$. *Given by*

$$\hat{a}_- = \frac{1}{\sqrt{2\hbar m\omega}}[i\hat{\vec{p}} + m\omega\hat{\vec{x}}]$$

- **Number operator**: The operator defined as follows. *Denoted by* $\boldsymbol{a}_+\boldsymbol{a}_-$. *Given by*

$$a_+a_- = \hat{a}_+ \circ \hat{a}_- = \frac{1}{2\hbar m\omega}\left[\hat{\vec{p}}^{\,2} + m^2\omega^2x^2 - im\omega[\hat{\vec{p}}, \hat{\vec{x}}]\right]$$

- Properties of these operators.
  - We can express $\hat{\vec{p}}, \hat{\vec{x}}$ in terms of a_+, a_- via

$$\hat{\vec{p}} = i\sqrt{\frac{\hbar m\omega}{2}}(\hat{a}_+ - \hat{a}_-) \qquad \hat{\vec{x}} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}_+ + \hat{a}_-)$$

    - It follows that

$$[\hat{\vec{p}}, \hat{\vec{x}}] = \frac{i\hbar}{2}[a_+ - a_-, a_+ + a_-] = \frac{i\hbar}{2}([a_+, a_-] - [a_-, a_+]) = i\hbar[a_+, a_-]$$

    - Consequently, since $[\hat{\vec{p}}, \hat{\vec{x}}] = -i\hbar$, we have that

$$[a_+, a_-] = -1$$

    - We also have that

$$[a_-, a_+] = 1$$

  - Since $[\hat{\vec{p}}, \hat{x}] = -i\hbar$ and $\omega^2 = k/m$, we have that

$$\begin{aligned}
a_+a_- &= \frac{1}{2\hbar m\omega}\left[\hat{\vec{p}}^{\,2} + m^2\omega^2x^2 - m\hbar\omega\right] \\
&= \frac{1}{\hbar\omega}\left[\underbrace{\frac{\hat{\vec{p}}^{\,2}}{2m} + \frac{kx^2}{2}}_{\hat{H}} - \frac{\hbar\omega}{2}\right] \\
\hat{H} &= \hbar\omega\left(a_+a_- + \frac{1}{2}\right)
\end{aligned}$$

- Because of the properties of $[a_+, a_-]$ proven above, we similarly have that

$$\hat{H} = \hbar\omega\left(a_-a_+ - \frac{1}{2}\right)$$

- We can also derive this equation in a manner exactly analogous to the first one.

- How does the number operator act on the eigenstate $|\psi_n\rangle$ of the harmonic oscillator?
  - Since $E_n = \hbar\omega(n + 1/2)$, we have that

$$\begin{aligned}
\hbar\omega\left(a_+a_- + \frac{1}{2}\right)|\psi_n\rangle &= \hat{H}|\psi_n\rangle \\
\hbar\omega\left(a_+a_- + \frac{1}{2}\right)|\psi_n\rangle &= \hbar\omega\left(n + \frac{1}{2}\right)|\psi_n\rangle \\
a_+a_-|\psi_n\rangle &= n|\psi_n\rangle
\end{aligned}$$

- How do the raising and lowering operators act on the eigenstate $|\psi_n\rangle$ of the harmonic oscillator?
  - Using a number of the above substitutions, we have that

$$\begin{aligned}
\hat{H}(a_+|\psi_n\rangle) &= \left[\hbar\omega\left(a_+a_- + \frac{1}{2}\right)\right](a_+|\psi_n\rangle) \\
&= \hbar\omega\left(a_+a_-a_+ + \frac{1}{2}a_+\right)|\psi_n\rangle \\
&= \hbar\omega a_+\left(a_-a_+ + \frac{1}{2}\right)|\psi_n\rangle \\
&= \hbar\omega a_+\left(a_+a_- + 1 + \frac{1}{2}\right)|\psi_n\rangle \\
&= \hbar\omega a_+\left(n + 1 + \frac{1}{2}\right)|\psi_n\rangle \\
&= E_{n+1}(a_+|\psi_n\rangle)
\end{aligned}$$

  - This means that $\hat{H}$ acts on $a_+|\psi_n\rangle$ the same way it acts on $|\psi_{n+1}\rangle$. In other words, it must be that

$$a_+|\psi_n\rangle \propto |\psi_{n+1}\rangle$$

  - Similarly,

$$\hat{H}(a_-|\psi_n\rangle) = E_{n-1}(a_-|\psi_n\rangle)$$

    so

$$a_-|\psi_n\rangle \propto |\psi_{n-1}\rangle$$

  - These actions are why a_+, a_- are called the *raising* and *lowering* operators!
  - We now seek to determine the constants of proportionality.
  - First off, note that a_+ and a_- are adjoints, i.e.,

$$a_+^\dagger = a_-$$

    - See Section 2.3 of Griffiths and Schroeter (2018) for a proof of this fact.
  - Then for a_+, we know that if

$$a_+|\psi_n\rangle = c_+|\psi_n\rangle$$

then

$$\begin{aligned}
c_+^2 &= c_+^2 \langle \psi_{n+1} | \psi_{n+1} \rangle \\
&= \langle c_+\psi_{n+1} | c_+\psi_{n+1} \rangle \\
&= \langle a_+\psi_n | a_+\psi_n \rangle \\
&= \langle \psi_n | a_+^\dagger a_+ | \psi_n \rangle \\
&= \langle \psi_n | a_- a_+ | \psi_n \rangle \\
&= \langle \psi_n | a_+ a_- + 1 | \psi_n \rangle \\
&= (n+1) \langle \psi_n | \psi_n \rangle \\
&= n+1
\end{aligned}$$

so that, taking square roots,

$$c_+ = \sqrt{n+1}$$

- By the same method — namely

$$c_-^2 = \langle a_-\psi_n | a_-\psi_n \rangle = \langle \psi_n | a_+ a_- | \psi_n \rangle = n$$

we can also learn that

$$c_- = \sqrt{n}$$

- Therefore,

$$a_+ |\psi_n\rangle = \sqrt{n+1}\, |\psi_{n+1}\rangle \qquad\qquad a_- |\psi_n\rangle = \sqrt{n}\, |\psi_{n-1}\rangle$$

- Note that what we have done here to derive this fact is far more slick than working directly with the unintuitive and complicated formal definitions of a_+, a_-.

- Now is a good time to mention a bit more about Dirac notation.
  - A "ket" represents a vector in a Hilbert space, so $|\psi_n\rangle$ demonstrates that we are talking about the wave function as a vector in the abstract linear algebra sense, not as a function $\psi_n : \mathbb{R}^4 \to \mathbb{C}$.
  - A "bra" represents a linear functional on a Hilbert space. In quantum mechanics, the linear functional $\langle \eta |$ is given by

$$\langle \eta | := \int \mathrm{d}^3\vec{r}\, \eta^*$$

  - Observe that this "functional" does indeed map any $|\psi_n\rangle$ given to it as an argument to a number $\langle \eta | \psi_n \rangle$!

- $|\psi_n\rangle$ can be defined in terms of a_+, $|\psi_0\rangle$, and constants.
  - Observe that since $a_+ |\psi_0\rangle = |\psi_1\rangle$ and $a_+ |\psi_1\rangle = \sqrt{2}\, |\psi_2\rangle$, we have that

$$|\psi_2\rangle = \frac{a_+}{\sqrt{2}} |\psi_1\rangle = \frac{a_+^2}{\sqrt{2}} |\psi_0\rangle$$

  - Similarly,

$$|\psi_3\rangle = \frac{a_+}{\sqrt{3}} |\psi_2\rangle = \frac{a_+^3}{\sqrt{3 \cdot 2}} |\psi_0\rangle$$

  - Generalizing, we have that

$$|\psi_n\rangle = \frac{a_+^n}{\sqrt{n!}} |\psi_0\rangle$$

- Thus, we have that

$$\psi_n(x) = \left(\frac{1}{\sqrt{2\hbar m\omega}}\right)^n \frac{1}{\sqrt{n!}} \left(-\hbar\frac{\mathrm{d}}{\mathrm{d}x} + xm\omega\right)^n \psi_0(x)$$

  where we may recall that

$$\psi_0(x) = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \mathrm{e}^{-m\omega x^2/2\hbar}$$

- Final observations about the raising and lowering operators.
  - Since $a_- |\psi_0\rangle = 0$ (as we may readily verify by direct computation), we have that

$$\hbar\frac{\mathrm{d}\psi_0}{\mathrm{d}x} + m\omega x\psi_0 = 0$$

  - We also know that

$$\mathrm{d}(\ln(\psi_0)) = -\frac{m\omega}{\hbar}\frac{\mathrm{d}x^2}{2}$$

    so

$$\psi_0 \propto \mathrm{e}^{-m\omega x^2/2\hbar}$$

    - What is the point of this line?? What new information does it give us?

- Raising and lowering operators allow us to compute the kinetic and potential energy of the harmonic oscillator.
  - Kinetic energy.

$$\begin{aligned}
\left\langle \psi_n \middle| \frac{\hat{\vec{p}}^2}{2m} \middle| \psi_n \right\rangle &= -\frac{\hbar\omega}{4} \langle\psi_n|(a_+ - a_-)^2|\psi_n\rangle \\
&= -\frac{\hbar\omega}{4} \langle\psi_n|a_+^2 + a_-^2 - a_+a_- - a_-a_+|\psi_n\rangle \\
&= -\frac{\hbar\omega}{4} [\underbrace{\langle\psi_n|a_+^2|\psi_n\rangle}_{\propto\langle\psi_n|\psi_{n+2}\rangle} + \underbrace{\langle\psi_n|a_-^2|\psi_n\rangle}_{\propto\langle\psi_n|\psi_{n-2}\rangle} - \underbrace{2\langle\psi_n|a_+a_-|\psi_n\rangle}_{2n\langle\psi_n|\psi_n\rangle} - \underbrace{\langle\psi_n|1|\psi_n\rangle}_{\langle\psi_n|\psi_n\rangle}] \\
&= \frac{\hbar\omega}{4}(2n+1) \\
&= \frac{\hbar\omega}{2}\left(n + \frac{1}{2}\right) \\
&= \frac{E_n}{2}
\end{aligned}$$

  - Potential energy.

$$\begin{aligned}
\langle\psi_n|\hat{H}|\psi_n\rangle &= E_n \\
\left\langle \psi_n \middle| \frac{\hat{\vec{p}}^2}{2m} \middle| \psi_n \right\rangle + \left\langle \psi_n \middle| \frac{k\hat{\vec{x}}^2}{2} \middle| \psi_n \right\rangle &= \frac{E_n}{2} + \frac{E_n}{2} \\
\left\langle \psi_n \middle| \frac{k\hat{\vec{x}}^2}{2} \middle| \psi_n \right\rangle &= \frac{E_n}{2}
\end{aligned}$$

  - Implication: In an energy eigenstate, the harmonic oscillator has equal values of kinetic and potential energies!

- Computing more observables.
  - We can show that
$$\langle\psi_n|\hat{\vec{x}}|\psi_n\rangle = \langle\psi_n|\hat{\vec{p}}|\psi_n\rangle = 0 \qquad \langle\psi_n|\hat{\vec{x}}^{\,2}|\psi_n\rangle = \frac{\hbar\omega}{k}\left(n+\frac{1}{2}\right) \qquad \langle\psi_n|\hat{\vec{p}}^{\,2}|\psi_n\rangle = \hbar\omega m\left(n+\frac{1}{2}\right)$$
- It follows from the above computations and the facts that
$$\Delta x^2 = \langle\psi_n|\hat{\vec{x}}^{\,2}|\psi_n\rangle - (\langle\psi_n|\hat{\vec{x}}|\psi_n\rangle)^2 \qquad \Delta p^2 = \langle\psi_n|\hat{\vec{p}}^{\,2}|\psi_n\rangle - (\langle\psi_n|\hat{\vec{p}}|\psi_n\rangle)^2$$
  that
$$\Delta x^2\cdot\Delta p^2 = \hbar^2\left(n+\frac{1}{2}\right)^2$$
$$\Delta x\cdot\Delta p = \frac{\hbar}{2}(2n+1)$$
  - Implication: The ground state $\psi_0(x)$ is represented by a Gaussian since in this case, $\Delta x\cdot\Delta p = \hbar/2$.
- Review from last class.
  - Mostly stuff I already wrote down.
  - One new equation formalizing the even/odd solutions:
$$f_n(x) = (-1)^n f_n(-x)$$
  - The first four Hermite polynomials:
$$H_0(\xi) = 1 \qquad H_1(\xi) = 2\xi \qquad H_2(\xi) = 4\xi^2 - 2 \qquad H_3 = 8\xi^3 - 12\xi$$
  - Summary of the characteristics of E_n: The energy is quantized and grows linearly with n in quanta of $\hbar\omega$, and has a minimum value $\hbar\omega/2$.
  - As with other time-independent potentials, the general solution to the Schrödinger equation will be
$$\psi(x,t) = \sum_n c_n\psi_n(x)\mathrm{e}^{-iE_nt/\hbar}$$
    where
$$\langle\psi|\hat{H}|\psi\rangle = \sum_n |c_n|^2E_n$$

4.2 Time Dependence and Coherent States

1/24: - Review of the harmonic oscillator.
  - Our Hamiltonian is
$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{kx^2}{2} = \frac{\hat{\vec{p}}^{\,2}}{2m} + \frac{k\hat{\vec{x}}^{\,2}}{2}$$
    - We have an analogy with the classical $\omega^2 = k/m$.
  - Under this Hamiltonian, $\hat{H}\,|\psi_n\rangle = E_n\,|\psi_n\rangle$ implies that
$$E_n = \hbar\omega\left(\frac{1}{2}+n\right)$$
  - The raising and lowering operators are given by
$$a_+ = \frac{1}{\sqrt{2\hbar m\omega}}[-i\hat{\vec{p}} + m\omega\hat{\vec{x}}] \qquad a_- = \frac{1}{\sqrt{2\hbar m\omega}}[i\hat{\vec{p}} + m\omega\hat{\vec{x}}]$$

- Together, these imply that

$$\hat{H} = \hbar\omega\left(a_+a_- + \frac{1}{2}\right)$$

- We also have that

$$a_+a_-\left|\psi_n\right\rangle = n\left|\psi_n\right\rangle \qquad a_+\left|\psi_n\right\rangle = \sqrt{n+1}\left|\psi_{n+1}\right\rangle$$
$$[a_-, a_+] = 1 \qquad a_-\left|\psi_n\right\rangle = \sqrt{n}\left|\psi_{n-1}\right\rangle$$

- We call a_+a_- the number operator.
- We should go home and learn these formulas.

– The full eigenstate is

$$\psi(x,t) = \sum_{n=0}^{\infty}\underbrace{c_n\psi_n(x)\mathrm{e}^{-iE_nt/\hbar}}_{\psi_n(x,t)}$$

– Two properties of this eigenstate.

1. We have that

$$\left|\psi\right\rangle = \sum_{n=0}^{\infty} c_n\mathrm{e}^{-iE_nt/\hbar}\left|\psi_n\right\rangle$$

which implies that

$$\sum_{n=0}^{\infty}|c_n|^2 = 1$$

since $\langle\psi|\psi\rangle = 1$ and $\langle\psi_n|\psi_m\rangle = \delta_{nm}$.

2. We have that

$$\langle\psi|\hat{H}|\psi\rangle = \sum_{n=0}^{\infty}|c_n|^2E_n$$

– We have that

$$\left\langle\psi_n\left|\frac{k\hat{\vec{x}}^2}{2}\right|\psi_n\right\rangle = \frac{\hbar\omega}{2}\left(n+\frac{1}{2}\right) = \frac{E_n}{2} \qquad \left\langle\psi_n\left|\frac{\hat{\vec{p}}^2}{2m}\right|\psi_n\right\rangle = \frac{\hbar\omega}{2}\left(n+\frac{1}{2}\right) = \frac{E_n}{2}$$

- Note that this makes sense because the sum $E_n/2 + E_n/2$ of potential and kinetic should be E_n, and it will be!

– Additionally, recall that we have

$$\hat{\vec{p}}^2 \propto (a_+ - a_-)^2 \qquad \hat{\vec{x}}^2 \propto (a_+ + a_-)^2$$

- Thus, we have that

$$\langle\psi_n|\hat{\vec{p}}|\psi_n\rangle = \langle\psi_n|(a_+ - a_-)|\psi_n\rangle = 0 \qquad \langle\psi_n|\hat{\vec{x}}|\psi_n\rangle = \langle\psi_n|(a_+ + a_-)|\psi_n\rangle = 0$$

– The harmonic oscillator is a very important problem in physics, and we should know it by heart! (In order to pass the class.)

- Recall as well that there is a correspondence between the Dirac notation and the functional notation, given by

$$\psi_n(x) \mapsto \left|\psi_n\right\rangle$$

– As an additional example,

$$\frac{1}{\sqrt{2\hbar m\omega}}\left[-\hbar\frac{\mathrm{d}}{\mathrm{d}x} + m\omega x\right]\psi_n(x) = \sqrt{n+1}\psi_{n+1}(x) \quad \mapsto \quad a_+\left|\psi_n\right\rangle = \sqrt{n+1}\left|\psi_{n+1}\right\rangle$$

- One more example:

$$\hbar\frac{\mathrm{d}\psi_0}{\mathrm{d}x}+m\omega x\psi_0(x)=0 \quad\mapsto\quad a_-\left|\psi_0\right\rangle=0$$

  - Note that solving this ODE yields the solution

$$\psi_0=C\exp\left(-\frac{m\omega x^2}{2\hbar}\right)$$

  - It appears that this is how we intuitively derive the ansatz we used last Friday!

- Now we start on some new content.
- Observe that

$$\begin{aligned}\frac{2m\omega\hat{\vec{x}}}{\sqrt{2\hbar m\omega}}&=a_++a_-\\ \hat{\vec{x}}&=\sqrt{\frac{\hbar}{2m\omega}}(a_++a_-)\end{aligned}$$

- In classical mechanics, the solution to the harmonic oscillator is

$$x(t)=A\sin\omega t+B\cos\omega t$$

- We now investigate the observables of $|\psi\rangle$.
- To start with, we show how $\langle\psi|\hat{\vec{x}}|\psi\rangle$ varies with time. This will lead into a discussion of something called coherent states. Let's begin.
  - We start with

$$\langle\psi|\hat{\vec{x}}|\psi\rangle=\sum_{m,n=0}^{\infty}c_m^*c_n\mathrm{e}^{i(E_m-E_n)t/\hbar}\left\langle\psi_m|\hat{\vec{x}}|\psi_n\right\rangle$$

  - We can algebraically manipulate the above to

$$\begin{aligned}\langle\psi|\hat{\vec{x}}|\psi\rangle&=\sum_{m,n=0}^{\infty}c_m^*c_n\mathrm{e}^{i(\hbar\omega(m-n))t/\hbar}\sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n+1}\delta_{m,n+1}+\sqrt{n}\delta_{m,n-1}\right)\\ &=\sum_{n=0}^{\infty}c_{n+1}^*c_n\mathrm{e}^{i\omega t}\sqrt{\frac{\hbar}{2m\omega}}\sqrt{n+1}+\sum_{n=1}^{\infty}c_{n-1}^*c_n\mathrm{e}^{-i\omega t}\sqrt{\frac{\hbar}{2m\omega}}\sqrt{n}\\ &=\sum_{n=0}^{\infty}c_{n+1}^*c_n\mathrm{e}^{i\omega t}\sqrt{\frac{\hbar}{2m\omega}}\sqrt{n+1}+\sum_{n=0}^{\infty}c_n^*c_{n+1}\mathrm{e}^{-i\omega t}\sqrt{\frac{\hbar}{2m\omega}}\sqrt{n+1}\\ &=\sqrt{\frac{\hbar}{2m\omega}}\cos(\omega t)\left[\sum_{n=0}^{\infty}\left(c_{n+1}^*c_n+c_n^*c_{n+1}\right)\sqrt{n+1}\right]\\ &\quad+\sqrt{\frac{\hbar}{2m\omega}}\sin(\omega t)\left[\sum_{n=0}^{\infty}\left(c_{n+1}^*c_n-c_n^*c_{n+1}\right)\sqrt{n+1}\right]\end{aligned}$$

  - Thus,

$$\langle\psi|\hat{\vec{x}}|\psi\rangle=A\cos\omega t+B\sin\omega t$$

    where

$$\begin{aligned}A&=2\operatorname{Re}\left[\sum_{n=0}^{\infty}c_{n+1}^*c_n\sqrt{n+1}\right]\sqrt{\frac{\hbar}{2m\omega}} & B&=2\operatorname{Im}\left[\sum_{n=0}^{\infty}c_{n+1}^*c_n\sqrt{n+1}\right]\sqrt{\frac{\hbar}{2m\omega}}\\ &=\operatorname{Re}\left[\sum_{n=0}^{\infty}c_{n+1}^*c_n\sqrt{n+1}\right]\sqrt{\frac{2\hbar}{m\omega}} & &=\operatorname{Im}\left[\sum_{n=0}^{\infty}c_{n+1}^*c_n\sqrt{n+1}\right]\sqrt{\frac{2\hbar}{m\omega}}\end{aligned}$$

- Now for large values of n,

$$\sqrt{n+1}\sqrt{\frac{2\hbar}{m\omega}} = \sqrt{\frac{2\hbar\omega(n+1)}{m\omega^2}} \approx \sqrt{\frac{2E_n}{m\omega^2}}$$

where

$$E_n = \hbar\omega\left(n+\frac{1}{2}\right) \qquad x = A\sin\omega t \qquad E = \frac{m\omega^2 A^2}{2} \qquad A = \sqrt{\frac{2E}{m\omega^2}}$$

  - How can we just ignore the real and imaginary sum terms??
- Now take the harmonic oscillator. Notice that $\sum_n$ is dominated by large values of $n \approx \bar{n}$, close to $\bar{n}$, where $\bar{n} \gg 1$. Thus,

$$\langle\psi|\hat{\vec{x}}|\psi\rangle = \sqrt{\frac{2E\bar{n}}{m\omega^2}} \sum_{n=0}^{\infty} \mathrm{Re}\left[\sum c_{n+1}^* c_n\right] \sin\omega t$$

and

$$\langle\psi|\hat{\vec{x}}^{\,2}|\psi\rangle - (\langle\psi|\hat{\vec{x}}|\psi\rangle)^2 \neq 0$$

- This is *not* classical motion.
- The states that come closest to realizing classical motion are called **coherent states**.

- **Coherent state** (of the harmonic oscillator): A state in which the uncertainty in $\hat{\vec{x}}$ is minimized. *Denoted by* $|\boldsymbol{\alpha}\rangle$.
- It turns out that the coherent states of the harmonic oscillator are the eigenstates of the lowering operator. Denoting the corresponding eigenvalue by α, we have that

$$a_- |\alpha\rangle = \alpha |\alpha\rangle$$

- Aside: $|\alpha\rangle$ can surely be expressed as a linear combination of the ψ_n. What does the lowering operator do to ψ_0, in particular, should it have a nonzero coefficient?
  - It acts as follows, simply zeroing it out.

$$a_- |\psi_0\rangle = 0\,|\psi_0\rangle$$

- Now what is $|\alpha\rangle$?
- Well, for a state to be coherent, we must have

$$\begin{aligned}
\frac{\hbar}{2} &= \sigma_x^2 \\
&= \langle\alpha|\hat{\vec{x}}^{\,2}|\alpha\rangle - (\langle\alpha|\hat{\vec{x}}|\alpha\rangle)^2 \\
&= \frac{\hbar}{2m\omega}\left[\langle\alpha|(a_+ + a_-)^2|\alpha\rangle - (\langle\alpha|(a_+ + a_-)|\alpha\rangle)^2\right] \\
&= \frac{\hbar}{2m\omega}\left[\langle\alpha|a_+^2 + a_+a_- + a_-a_+ + a_-^2|\alpha\rangle - (\langle\alpha|(a_+ + a_-)|\alpha\rangle)^2\right] \\
&= \dots
\end{aligned}$$

  - We'll finish this up next time.
  - Is it really $\hbar/2$ here??

4.3 Hermitian Operators; Position and Momentum Eigenstates

1/26:
- Recap of the harmonic oscillator.
  - The Hamiltonian (in terms of $\hat{p}, \hat{x}$; and in terms of a_+, a_-).
  - The definitions of a_+, a_-.
  - The effect of a_+, a_- on $|n\rangle := |\psi_n\rangle$.
  - The effect of $\hat{H}$ on $|n\rangle$.
  - Adjoints of the **ladder operators**:

$$(a_+)^\dagger = a_- \qquad\qquad (a_-)^\dagger = a_+$$

  - The commutator $[a_-, a_+] = 1$.
  - The formula for a generic state $|\psi\rangle$, i.e.,

$$|\psi\rangle = \sum_{n=0}^{\infty} c_n \mathrm{e}^{-iE_n t/\hbar} |n\rangle$$

    - This will of course appear as a question in the midterm and final!
    - We must also remember that

$$1 = \langle\psi|\psi\rangle = \sum_{n=0}^{\infty} |c_n|^2 \qquad\qquad 1 = \langle\psi|\hat{H}|\psi\rangle = \sum_{n=0}^{\infty} |c_n|^2 E_n$$

  - The probability of measuring the energy of $|\psi\rangle$ as E_n is $|c_n|^2$.
    - So when we perform a measurement, the energy of $|\psi\rangle$ collapses to that of one eigenstate.
- **Ladder operator**: An element in the class of operators that send $|n\rangle$ to scalar multiples of $|n+i\rangle$ for some $i \in \mathbb{Z} \setminus \{0\}$.
  - The raising and lowering operators are ladder operators!
- The midterm.
  - 50% of the midterm will be related to harmonic oscillator content, esp. the last few equations above following the definition of $|\psi\rangle$.
  - The midterm will only cover what we covered through today.
  - The midterm may be on February 5. It sounds like it will be on Friday, February 9, though.
  - It will take place in this classroom.
  - It will be open book.
    - Can we bring virtual notes, or does everything have to be printed out??
  - The midterm questions will be the same level as the PSet questions; there may even be some repetition! Def take a look at the PSets.
  - PSet 1 through PSet 4 will be covered on the midterm.
  - Foundations of quantum mechanics plus one-dimensional problems.
  - We will be allowed to turn in the midterm through 1:00 PM, though it shouldn't take us more than 50 minutes.
- The first two problems of PSet 4 must be solved; the third one can be dropped *or* can be solved for 5 bonus points.
- We now begin on new content.

- Recall the following expression from last class.

$$\langle\psi|\hat{\vec{x}}|\psi\rangle = \sqrt{\frac{2\hbar}{m\omega}}\sum_{n=0}^{\infty}\left[\sqrt{n+1}\cos(\omega t)\operatorname{Re}(c_{n+1}^{*}c_n) + \sqrt{n+1}\sin(\omega t)\operatorname{Im}(c_{n+1}^{*}c_n)\right]$$

  - This is a really complicated expression, especially as we prepare to talk about coherent states.
  - Thus, it was quite difficult to prove that

$$\langle\psi|\hat{\vec{x}}^{\,2}|\psi\rangle \neq (\,\langle\psi|\hat{\vec{x}}|\psi\rangle)^2$$

  - Can we introduce a notation that will allow us to work with this expression and similar ones more easily?
- Wagner restates the definition of a coherent state and and the uncertainty principles.
- Recall that

$$a_-\,|\alpha\rangle = \alpha\,|\alpha\rangle$$

  and that

$$|\alpha\rangle = \sum_n c_n\,|n\rangle$$

- The Hermitian conjugate of a_- is a_+ and hence, the Hermitian conjugate of $a_-\,|\alpha\rangle$ is

$$\langle\alpha|\,a_+ = \langle\alpha|\,\alpha^*$$

- Thus, since $\langle\alpha|\alpha\rangle = 1$

$$\langle\alpha|a_+a_-|\alpha\rangle = \alpha\,\langle\alpha|a_+|\alpha\rangle = \alpha\,\langle\alpha|\alpha^*|\alpha\rangle = \alpha^*\alpha\,\langle\alpha|\alpha\rangle = \alpha^*\alpha$$

- We now seek to verify that an eigenstate of a_- does, in fact, minimize the uncertainty in $\hat{x}$.
  - For simplicity, we will consider $|\alpha\rangle$ at $t = 0$ (this will remove the complex exponential from calculations).
  - First off, we have that

$$\langle\alpha|\hat{\vec{x}}|\alpha\rangle = \sqrt{\frac{\hbar}{2m\omega}}\,\langle\alpha|(a_+ + a_-)|\alpha\rangle = (\alpha^* + \alpha)\sqrt{\frac{\hbar}{2m\omega}}$$

  and

$$\begin{aligned}\langle\alpha|\hat{\vec{x}}^{\,2}|\alpha\rangle &= \frac{\hbar}{2m\omega}\,\langle\alpha|(a_+ + a_-)(a_+ + a_-)|\alpha\rangle\\ &= \frac{\hbar}{2m\omega}[\,\langle\alpha|a_+^2|\alpha\rangle + \,\langle\alpha|a_+a_-|\alpha\rangle + \,\langle\alpha|a_-a_+|\alpha\rangle + \,\langle\alpha|a_-^2|\alpha\rangle]\\ &= \frac{\hbar}{2m\omega}[(\alpha^*)^2\underbrace{\langle\alpha|\alpha\rangle}_{1} + \alpha^*\alpha + \,\langle\alpha|(\underbrace{a_-a_+ - a_+a_-}_{1} + a_+a_-)|\alpha\rangle + \alpha^2]\\ &= \frac{\hbar}{2m\omega}[(\alpha^*)^2 + \alpha^2 + 2|\alpha|^2 + 1]\end{aligned}$$

  - Combining these, we have that

$$\langle\alpha|\hat{\vec{x}}^{\,2}|\alpha\rangle - (\,\langle\alpha|\hat{\vec{x}}|\alpha\rangle)^2 = \frac{\hbar}{2m\omega}[(\alpha^*)^2 + \alpha^2 + 2|\alpha|^2 + 1 - (\alpha^*)^2 - \alpha^2 - 2|\alpha|^2] = \frac{\hbar}{2m\omega}$$

- Second, we have that

$$\langle\alpha|\hat{\vec{p}}|\alpha\rangle = \sqrt{\frac{\hbar m\omega}{2}}\,\langle\alpha|(a_+ - a_-)|\alpha\rangle = \sqrt{\frac{\hbar m\omega}{2}}(\alpha^* - \alpha)$$

and

$$\begin{aligned}\langle\alpha|\hat{\vec{p}}^2|\alpha\rangle &= -\frac{\hbar m\omega}{2}\,\langle\alpha|(a_+ - a_-)(a_+ - a_-)|\alpha\rangle\\ &= -\frac{\hbar m\omega}{2}\left[(\alpha^*)^2 + \alpha^2 - |\alpha|^2 - \langle\alpha|\underbrace{a_-a_+}_{a_+a_-+1}|\alpha\rangle\right]\\ &= -\frac{\hbar m\omega}{2}\left[(\alpha^*)^2 + \alpha^2 - 2|\alpha|^2 - 1\right]\end{aligned}$$

- Combining these, we have that

$$\langle\alpha|\hat{\vec{p}}^2|\alpha\rangle - (\langle\alpha|\hat{\vec{p}}|\alpha\rangle)^2 = \frac{\hbar m\omega}{2}\left[-(\alpha^*)^2 - \alpha^2 + 2|\alpha|^2 + 1 + (\alpha^*)^2 + \alpha^2 - 2|\alpha|^2\right] = \frac{\hbar m\omega}{2}$$

- Therefore,

$$\begin{aligned}\sigma_p^2\sigma_x^2 &= \frac{\hbar m\omega}{2}\cdot\frac{\hbar}{2m\omega}\\ &= \frac{\hbar^2}{4}\\ \sigma_p\sigma_x &= \frac{\hbar}{2}\end{aligned}$$

as desired.

- If we reassert full time dependence, we obtain

$$|\alpha\rangle(t) = \sum_n c_n \mathrm{e}^{-iE_nt/\hbar}|n\rangle$$

  - Then

$$\begin{aligned}a_-|\alpha\rangle &= \sum_{n=0}^{\infty} c_n \mathrm{e}^{-iE_nt/\hbar}\sqrt{n}\,|n-1\rangle\\ &= \sum_{n=0}^{\infty} c_{n+1}\mathrm{e}^{-iE_{n+1}t/\hbar}\sqrt{n+1}\,|n\rangle\end{aligned}$$

  - And recall that

$$a_-|\alpha\rangle = \alpha|\alpha\rangle$$

  - Thus, via term-by-term transitivity for each $|n\rangle$,

$$\begin{aligned}\alpha c_n &= c_{n+1}\mathrm{e}^{-i(E_{n+1}-E_n)t/\hbar}\sqrt{n+1}\\ \alpha c_n &= c_{n+1}\mathrm{e}^{-i\omega t}\sqrt{n+1}\end{aligned}$$

  - If α is real and $\psi_\alpha(x)$ denotes the time-independent factor in $|\alpha\rangle$, then

$$\begin{aligned}a_-\psi_\alpha(x) &= \alpha\psi_\alpha(x)\\ \left[\hbar\frac{\mathrm{d}}{\mathrm{d}x} + m\omega x\right]\psi_\alpha(x) &= \alpha\psi_\alpha(x)\end{aligned}$$

- Then
$$\frac{1}{\psi_\alpha}\frac{\mathrm{d}}{\mathrm{d}x}\psi_\alpha + \left(\frac{m\omega x}{\hbar} - \alpha\right) = 0$$
- Thus, solving the differential equation, we obtain
$$\psi_\alpha = \exp\left[-\frac{m\omega}{2\hbar}(x - \langle x\rangle)^2\right]$$
which is a Gaussian.
- Therefore,
$$a_- \left|0\right\rangle = 0 \left|0\right\rangle$$

- We will program the time evolution of a coherent state in Python or Mathematica??
  - A real wave function is a crazy thing that does flip from side to side at $T/2$ and T.
    - Essentially,
$$|\psi(x,t)|^2 = |\psi(-x,t+T/2)|^2$$
  - A coherent state is just a Gaussian that oscillates back and forth to both sides of the y-axis.

4.4 Chapter 2: Time-Independent Schrödinger Equation

From Griffiths and Schroeter (2018).

Section 2.3: The Harmonic Oscillator

1/29:
- Sets up the relevant TISE, as in class.
- Note that "it is customary to eliminate the spring constant in favor of the classical frequency" (Griffiths & Schroeter, 2018, p. 58).
- Goes through the ladder operator method in great detail and very coherently; I should probably return!!
  - There is a proof in here of why $a_+^\dagger = a_-$.
- Goes through the **power series method** from the Lecture 7 notes.
  - This is the brute force method, though it is useful (as with the hydrogen atom later on).
- **Canonical commutation relation**: The relation defined as follows. *Given by*
$$[\hat{x}, \hat{p}] = i\hbar$$

Section 2.4: The Free Particle

- Relevant to 1/5 and 1/17 discussions; I should probably return!!

Section 2.5: The Delta-Function Potential

- Relevant to PSet 2; I should probably return!!

Section 2.6: The Finite Square Well

- Relevant to PSet 2; I should probably return!!

4.5 Chapter 3: Formalism

From Griffiths and Schroeter (2018).

Section 3.1: Hilbert Space

- Purpose: Recast some of the miracles we've encountered thus far in more powerful terms.
- Lots of stuff I should read just for fun (tons of answers to questions I've wondered at over the years), and some stuff actually related to in-class discussions of Hermitian operators, compatible operators, proving the uncertainty principle, Gaussian wave packets, the Ehrenfest theorem, Dirac notation, etc.

4.6 Appendix: Linear Algebra

From Griffiths and Schroeter (2018).

- A terrific review of relevant concepts, all expressed in Dirac notation.

Week 5

Three-Dimensional Systems

5.1 Three-Dimensional Problems

1/29: • 3D problems still solve the Schrödinger equation, just in 3D.

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

  – Slightly more complicated here, but not too much.

• Focus: Time-independent potentials for now, that is

$$V(\vec{r},t) = V(\vec{r})$$

  – 3D time-independent potentials still allow us to split the wave function as on the left below, and we also still seek energy eigenvalues of the system on the right below.

$$\psi(\vec{r},t) = \psi(\vec{r})\cdot\phi(t) \qquad\qquad -\frac{\hbar^2}{2m}\vec{\nabla}^2\psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) = E\psi(\vec{r})$$

  – These two facts still imply that the solution will be of the form

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

    ■ No difference between 1D and 3D!

• So 1D and 3D are remarkably similar. But where do they differ?

• Example: In 3D, there will be 3 components of the momentum, given as follows.

$$\hat{p}_x = -i\hbar\frac{\partial}{\partial x} \qquad \hat{p}_y = -i\hbar\frac{\partial}{\partial y} \qquad \hat{p}_z = -i\hbar\frac{\partial}{\partial z}$$

  – Note that these three momenta commute as follows.

$$[\hat{p}_x,\hat{p}_y] = [\hat{p}_y,\hat{p}_z] = [\hat{p}_z,\hat{p}_x] = 0$$

• Example: 3 components of the position, also commutative.

$$[\hat{x},\hat{y}] = [f(\hat{x}),f(\hat{y})] = [f(\hat{x}),g(\hat{x})] = [f(\hat{x}),g(\hat{z})] = 0$$

  – As in PSet 4, f,g are arbitrary real functions of the operator.

- The only commutators that are not zero are those we obtained before, e.g.,
$$[\hat{p}_x,\hat{x}]=-i\hbar \qquad [\hat{\vec{p}},V(\vec{r})]=-i\hbar\vec{\nabla}V(\vec{r})$$
  - Recall that we still have
$$[\hat{p}_x,\hat{y}]=[\hat{p}_x,\hat{z}]=0 \qquad [V(\vec{r}),\hat{\vec{r}}]=0$$
- In the presence of $V(\vec{r})$, neither of $\hat{\vec{p}},\hat{x}$ are conserved quantities. We know this because
$$[\hat{H},\vec{p}]=[\hat{H},\vec{r}]\neq 0$$
- In an atom...
  - Potential is only a function of the *magnitude* of distance from the nucleus. Mathematically,
$$V(\vec{r})=V(r)$$
  - Likewise, angular momentum $\vec{L}=\vec{r}\times\vec{p}$ is conserved. Here's why:
    - Recall that
$$\begin{aligned}\frac{\mathrm{d}\vec{L}}{\mathrm{d}t}&=\frac{\mathrm{d}\vec{r}}{\mathrm{d}t}\times\vec{p}+\vec{r}\times\frac{\mathrm{d}\vec{p}}{\mathrm{d}t}\\&=\frac{1}{m}\underbrace{\vec{p}\times\vec{p}}_{0}+\vec{r}\times\underbrace{\frac{\mathrm{d}\vec{p}}{\mathrm{d}t}}_{-\vec{\nabla}V(r)}\end{aligned}$$
    - Working with the second term a bit more, we have that
$$\begin{aligned}\vec{\nabla}V(r)&=\vec{x}\frac{\partial V}{\partial x}+\vec{y}\frac{\partial V}{\partial y}+\vec{z}\frac{\partial V}{\partial z}\\&=\vec{x}\left(\frac{\partial V}{\partial r}\frac{\partial r}{\partial x}\right)+\vec{y}\left(\frac{\partial V}{\partial r}\frac{\partial r}{\partial y}\right)+\vec{z}\left(\frac{\partial V}{\partial r}\frac{\partial r}{\partial z}\right)\\&=\frac{\partial V}{\partial r}\left(\vec{x}\frac{\partial r}{\partial x}+\vec{y}\frac{\partial r}{\partial y}+\vec{z}\frac{\partial r}{\partial z}\right)\end{aligned}$$
      - Taking the cross product of the above (evaluated at $r=\sqrt{x^2+y^2+z^2}$) with $\vec{r}$ yields zero.
      - Alternatively, we may observe that like each $\partial V/\partial x\propto x$, we have $\vec{\nabla}V\propto\vec{r}$ for a central potential (just picture it), and therefore the cross product of $\vec{r}$ and a vector proportional to $\vec{r}$ will be zero.
    - Therefore,
$$\frac{\mathrm{d}\vec{L}}{\mathrm{d}t}=\frac{1}{m}\underbrace{\vec{p}\times\vec{p}}_{0}+\underbrace{\vec{r}\times c\vec{r}}_{0}=0$$
    so angular momentum is conserved, as desired.
- What does it mean that these two quantities are conserved?
  - It means that when we take the classical Hamiltonian
$$\hat{H}=\frac{\vec{p}^{\,2}}{2m}+V(r)$$
  we can separate it into a radial and a perpendicular component so that
$$\begin{aligned}\hat{H}&=\frac{\hat{p}_r^2}{2m}+\frac{\hat{p}_\perp^2}{2m}+V(r)\\&=\frac{\hat{p}_r^2}{2m}+\underbrace{\frac{\vec{L}^2}{2mr^2}+V(r)}_{V_{\text{eff}}(r)}\end{aligned}$$

- Here's why we can make the above algebraic manipulations.
  - To begin, we can always split the momentum operator into radial and perpendicular components.
  - We also know, since $\vec{p}_\perp$ and $\vec{r}$ are perpendicular, that

$$\vec{L}^2 = (\vec{p}_\perp \times \vec{r})^2 = [p_\perp r \sin(90°)]^2 = p_\perp^2 r^2 = \hat{p}_\perp^2 r^2$$

  - However, it is the conservation of angular momentum, in particular, which implies that $\vec{L}^2$ is a constant, and hence that making the substitution $\hat{p}_\perp^2 = \vec{L}^2/r^2$ will allow the sum of the second two terms to be *purely* a function of r (as opposed to, per se, a function of r and $\vec{L}$).
- What is the implication of this effective potential?

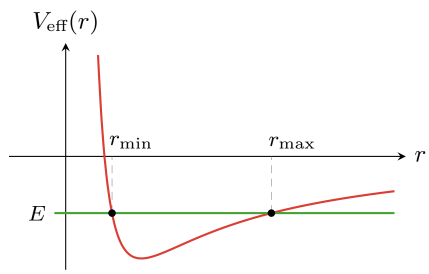


Figure 5.1: Effective potential.

  - Consider the classical case of planetary motion with

$$V_{\text{eff}}(r) = -\frac{GM_0m}{r} + \frac{\vec{L}^2}{2mr^2}$$

  - Given a total energy E for the system, the planets dance between an r_{min} and r_{max}.
  - This gives the elliptical planetary motion.
  - Of course, we will not deal with planetary motion in this course, but we will deal with something very similar called the **hydrogen atom**.
- We now investigate some analogies and differences between classical and quantum mechanics.
- Before we begin, a quick aside on some commutator rules will be useful.
  1. $[\hat{A}^2, \hat{B}] = \hat{A}[\hat{A}, \hat{B}] + [\hat{A}, \hat{B}]\hat{A}$.

     Proof.

$$\begin{aligned}
[\hat{A}^2, \hat{B}] &= \hat{A}^2\hat{B} - \hat{B}\hat{A}^2 \\
&= \hat{A}(\hat{A}\hat{B} - \hat{B}\hat{A}) + (\hat{A}\hat{B} - \hat{B}\hat{A})\hat{A} \\
&= \hat{A}[\hat{A}, \hat{B}] + [\hat{A}, \hat{B}]\hat{A}
\end{aligned}$$

□

  2. $[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}$.
  3. $[\hat{A}, \hat{B}\hat{C}] = \hat{B}[\hat{A}, \hat{C}] + [\hat{A}, \hat{B}]\hat{C}$.
  4. Bilinearity, i.e.,

$$\begin{aligned}
[\hat{A} + \hat{B}, \hat{C}] &= [\hat{A}, \hat{C}] + [\hat{B}, \hat{C}] & [c\hat{A}, \hat{B}] &= c[\hat{A}, \hat{B}] \\
[\hat{A}, \hat{B} + \hat{C}] &= [\hat{A}, \hat{B}] + [\hat{A}, \hat{C}] & [\hat{A}, c\hat{B}] &= c[\hat{A}, \hat{B}]
\end{aligned}$$

- None of these rules is trivial, but they can all be demonstrated by expanding as with the first rule.

- So getting back to it, the analogies and differences we will prove are...
  1. The quantum angular momentum is conserved directionally and overall;
  2. The square of the quantum angular momentum is conserved;
  3. The quantum angular momentum *cannot* be determined to infinite precision in more than one direction simultaneously;
  4. The square of the quantum angular momentum and the quantum angular momentum can be determined to infinite precision simultaneously.
- Task 1: To prove that the quantum angular momentum is conserved directionally, we will show that the angular momentum in different directions commutes with the Hamiltonian. To prove that it is conserved overall, we will add the previous three results. Let's begin.
  - Mathematically, we want to determine

    $$[\hat{H}, \hat{L}_i] \stackrel{?}{=} 0$$

    since if $[\hat{H}, \hat{L}_i] = 0$, then

    $$\frac{\mathrm{d}}{\mathrm{d}t}\Big(\langle\psi|\hat{L}_i|\psi\rangle \Big) = \frac{i}{\hbar} \langle\psi|\underbrace{[\hat{H}, \hat{L}_i]}_{0}|\psi\rangle = 0$$
  - Let's start with $\hat{L}_x$.
  - Since

    $$\vec{L} = \vec{r} \times \vec{p} = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix} = \hat{x}(yp_z - p_y z) + \hat{y}(p_x z - p_z x) + \hat{z}(xp_y - p_x y)$$

    we know that

    $$\hat{L}_x = yp_z - p_y z$$
  - Additionally, recall that

    $$\hat{H} = \frac{\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2}{2m} + V(r)$$
  - Thus, we have that

    $$\begin{aligned} [\hat{H}, \hat{L}_x] &= \left[\frac{\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2}{2m} + V(r), \hat{y}\hat{p}_z - \hat{z}\hat{p}_y \right] \\ &= \left[\frac{\hat{p}_x^2}{2m}, \hat{y}\hat{p}_z \right] + \left[\frac{\hat{p}_y^2}{2m}, \hat{y}\hat{p}_z \right] + \left[\frac{\hat{p}_z^2}{2m}, \hat{y}\hat{p}_z \right] \\ &\quad + \left[\frac{\hat{p}_x^2}{2m}, -\hat{z}\hat{p}_y \right] + \left[\frac{\hat{p}_y^2}{2m}, -\hat{z}\hat{p}_y \right] + \left[\frac{\hat{p}_z^2}{2m}, -\hat{z}\hat{p}_y \right] \\ &\quad + [V(r), \hat{y}\hat{p}_z] + [V(r), -\hat{z}\hat{p}_y] \\ &= \left[\frac{\hat{p}_y^2}{2m}, \hat{y}\hat{p}_z \right] + \left[\frac{\hat{p}_z^2}{2m}, -\hat{z}\hat{p}_y \right] + i\hbar \left(\hat{y}\frac{\partial V}{\partial z} - \hat{z}\frac{\partial V}{\partial y} \right) \\ &= -\frac{i\hbar\hat{p}_y\hat{p}_z}{m} + \frac{i\hbar\hat{p}_y\hat{p}_z}{m} + i\hbar\frac{\partial V}{\partial r} \left(\hat{y}\frac{\partial r}{\partial z} - \hat{z}\frac{\partial r}{\partial y} \right) \\ &= 0 \end{aligned}$$
  - Now let's investigate some of the above substitutions a bit more closely.
  - From line 1 to line 2, we split the commutator into $4 \cdot 2 = 8$ terms using its bilinearity.

- From line 2 to line 3, we eliminated all commutators that go to zero among the first six, and evaluated the last two commutators using a combination of Rule 3 and properties mentioned at the beginning of the lecture.
  - Notice that the only two of the first six commutators that did *not* go to zero were those for which the variable in the squared momentum operator matched the position operator, i.e., in

$$\left[\frac{\hat{p}_y^2}{2m},\hat{y}\hat{p}_z\right]$$

    we may observe that $\hat{p}_y^2$ and $\hat{y}$ both concern y.
  - Example evaluation:

$$\begin{aligned}
\left[\frac{\hat{p}_x^2}{2m},\hat{y}\hat{p}_z\right] &= \frac{1}{2m}[\hat{p}_x^2,\hat{y}\hat{p}_z] && \text{Rule 4}\\
&= \frac{1}{2m}(\hat{p}_x[\hat{p}_x,\hat{y}\hat{p}_z]+[\hat{p}_x,\hat{y}\hat{p}_z]\hat{p}_x) && \text{Rule 1}\\
&= \frac{1}{2m}(\hat{p}_x(\hat{y}\underbrace{[\hat{p}_x,\hat{p}_z]}_{0}+\underbrace{[\hat{p}_x,\hat{y}]}_{0}\hat{p}_z)+(\hat{y}\underbrace{[\hat{p}_x,\hat{p}_z]}_{0}+\underbrace{[\hat{p}_x,\hat{y}]}_{0}\hat{p}_z)\hat{p}_x) && \text{Rule 3}\\
&= 0
\end{aligned}$$

  - Example evaluation:

$$\begin{aligned}
\left[\frac{\hat{p}_y^2}{2m},\hat{y}\hat{p}_z\right] &= \frac{1}{2m}[\hat{p}_y^2,\hat{y}\hat{p}_z] && \text{Rule 4}\\
&= \frac{1}{2m}(\hat{p}_y[\hat{p}_y,\hat{y}\hat{p}_z]+[\hat{p}_y,\hat{y}\hat{p}_z]\hat{p}_y) && \text{Rule 1}\\
&= \frac{1}{2m}(\hat{p}_y(\hat{y}\underbrace{[\hat{p}_y,\hat{p}_z]}_{0}+\underbrace{[\hat{p}_y,\hat{y}]}_{-i\hbar}\hat{p}_z)+(\hat{y}\underbrace{[\hat{p}_y,\hat{p}_z]}_{0}+\underbrace{[\hat{p}_y,\hat{y}]}_{-i\hbar}\hat{p}_z)\hat{p}_y) && \text{Rule 3}\\
&= \frac{1}{2m}(\hat{p}_y(-i\hbar\hat{p}_z)+(-i\hbar\hat{p}_z)\hat{p}_y)\\
&= -\frac{i\hbar}{2m}(\hat{p}_y\hat{p}_z+\hat{p}_z\hat{p}_y)\\
&= -\frac{i\hbar}{2m}(\hat{p}_y\hat{p}_z+\hat{p}_y\hat{p}_z)\\
&= -\frac{i\hbar\hat{p}_y\hat{p}_z}{m}
\end{aligned}$$

    - Note that $\hat{p}_z\hat{p}_y=\hat{p}_y\hat{p}_z$ because $[\hat{p}_y,\hat{p}_z]=0$.
  - Example evaluation:

$$\begin{aligned}
[V(r),\hat{y}\hat{p}_z] &= \hat{y}\underbrace{[V(r),\hat{p}_z]}_{i\hbar\,\partial V/\partial z}+\underbrace{[V(r),\hat{y}]}_{0}\hat{p}_z && \text{Rule 3}\\
&= i\hbar\hat{y}\frac{\partial V}{\partial z}
\end{aligned}$$

- From line 3 to line 4, we evaluated the last two commutators and applied the chain rule.
- From line 4 to line 5, we algebraically expanded and cancelled everything (using $r=\sqrt{x^2+y^2+z^2}$ for the partial derivatives).
- Moving on, similar to the above, we obtain that

$$[\hat{H},\hat{L}_y]=[\hat{H},\hat{L}_z]=0$$

- Thus, by bilinearity once more,

$$[\hat{H},\hat{\vec{L}}]=[\hat{H},\hat{L}_x+\hat{L}_y+\hat{L}_z]=0$$

- Task 2: The fact that the Hamiltonian commutes with the constant $\hat{\vec{L}}^2$ is obvious, implying the claim.
- Task 3.
  - Here, we want to investigate if
  $$[L_x,L_y]\stackrel{?}{=}0$$
  - We do this via
  $$\begin{aligned}[L_x,L_y]&=[\hat{y}\hat{p}_z-\hat{z}p_y,p_xz-xp_z]\\&=[yp_z,p_xz]+[\hat{z}\hat{p}_y,\hat{x}\hat{p}_z]\\&=\hat{y}\hat{p}_x(-i\hbar)+\hat{p}_y\hat{x}(i\hbar)\\&=i\hbar\hat{L}_z\end{aligned}$$
  - Similarly, we can see that no $\hat{L}_i$'s commute with each other. Indeed, altogether, we have
  $$[\hat{L}_x,\hat{L}_y]=i\hbar\hat{L}_z\qquad[\hat{L}_y,\hat{L}_z]=i\hbar\hat{L}_x\qquad[\hat{L}_z,\hat{L}_x]=i\hbar\hat{L}_y$$
- Task 4.
  - We have that
  $$\begin{aligned}[\hat{\vec{L}}^2,\hat{L}_x]&=[\hat{L}_x^2+\hat{L}_y^2+\hat{L}_z^2,\hat{L}_x]\\&=0+[\hat{L}_y^2,\hat{L}_x]+[\hat{L}_z^2,\hat{L}_x]\\&=\hat{L}_y[\hat{L}_y,\hat{L}_x]+[\hat{L}_y,\hat{L}_x]\hat{L}_y+\hat{L}_z[\hat{L}_z,\hat{L}_x]+[\hat{L}_z,\hat{L}_x]\hat{L}_z\\&=\hat{L}_y(-i\hbar\hat{L}_z)+(-i\hbar\hat{L}_z)\hat{L}_y+\hat{L}_z(i\hbar\hat{L}_y)+(i\hbar\hat{L}_y)\hat{L}_z\\&=i\hbar(-\hat{L}_y\hat{L}_z-\hat{L}_z\hat{L}_y+\hat{L}_z\hat{L}_y+\hat{L}_y\hat{L}_z)\\&=0\end{aligned}$$
  - Thus, the squares commute:
  $$[\hat{\vec{L}}^2,\hat{L}_x]=[\hat{\vec{L}}^2,\hat{L}_y]=[\hat{\vec{L}}^2,\hat{L}_z]=0$$
- Conclusion.
  - $\hat{L}_i,\hat{\vec{L}}^2$ are conserved. That is,
  $$[\hat{H},\hat{L}_i]=[\hat{H},\hat{\vec{L}}^2]=0$$
    - This means that $\hat{H},\hat{L}_z,\hat{\vec{L}}^2$ have compatible observables.
    - In other words, we can only define the angular momentum in one direction and the modulus of the angular momentum squared.
  - All this will characterize three-dimensional motion as we'll see.

References

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