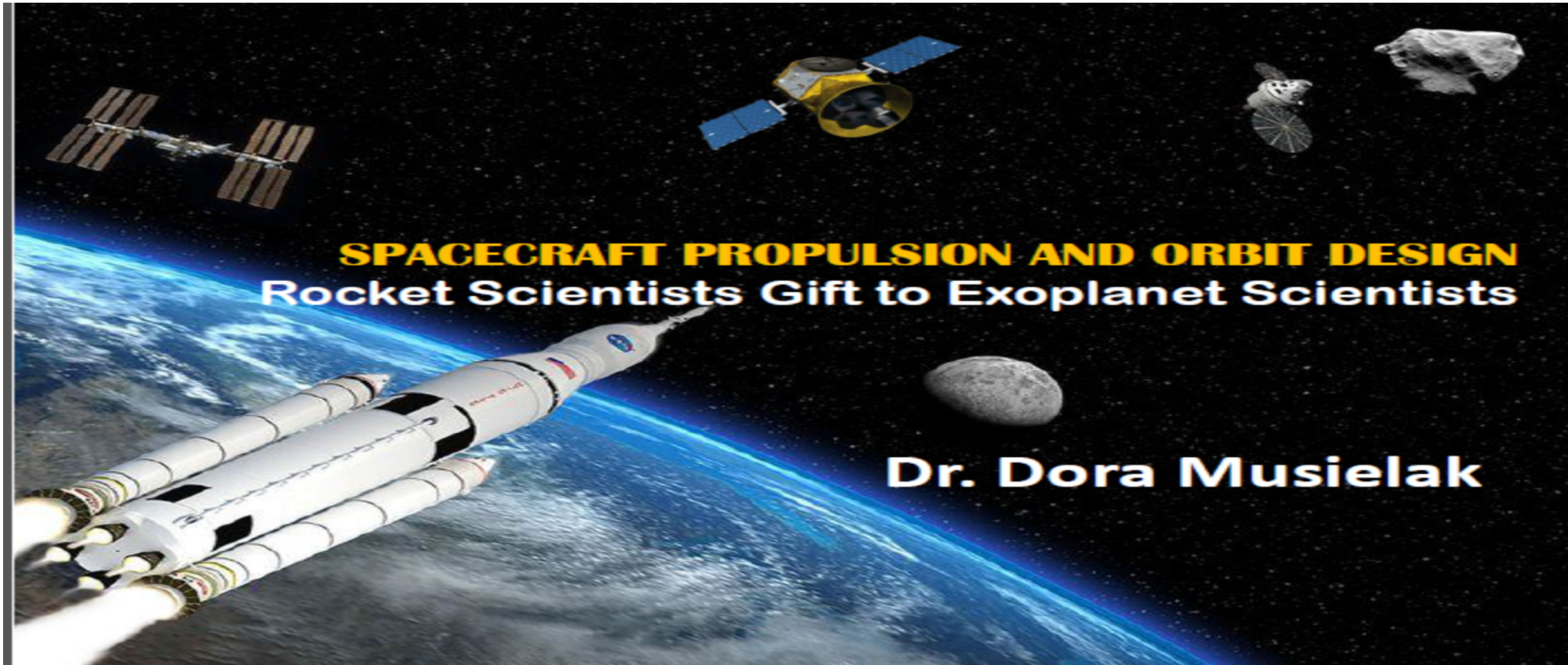
PHYS 3313 – Section 001
Lecture #18

Monday, April 1, 2019
Dr. Jaehoon Yu

- Time Independent Schrodinger Equation
- Expectation Values
- Momentum Operator
- Position and Energy Operators
- Infinite Square-well Potential

Announcements

- Bring out HW#4
- Quiz #3
  – Beginning of the class, Wednesday, Apr. 3
  – Covers: CH4.8 through what we finish Monday, Apr. 1
  – BYOF: You may bring a one 8.5x11.5 sheet (front and back) of handwritten formulae and values of constants for the exam
  – No derivations, word definitions or setups or solutions of any problems!
    - No Maxwell's equations!
  – No additional formulae or values of constants will be provided!
- A special colloquium at 4pm today in SH101
  – Dr. Dora Muesielak of UTA



Starting with an overview of rocket propulsion, I will introduce spacecraft trajectories in the Sun-Earth-Moon System, focusing especially on those appropriate for exoplanet hunting missions. One type of heliocentric orbit about a libration point, known as halo orbit, was selected for the Wide Field Infrared Survey Telescope (WFIRST) and the James Webb Space Telescope (JWST). The mission objectives of these spacecraft are to search for exoplanets while studying dark matter, and to study atmospheres of known exoplanets, respectively. Another unique spacecraft trajectory concept is the lunar-resonant High Earth Orbit (HEO) chosen for the Transiting Exoplanet Survey Satellite (TESS), whose mission objective is to examine over 85% of the sky, an area 400 times larger than what the Kepler telescope observed. I will also include a unique halo orbit on a radio-quiet zone located on the farside of the Moon.

MONDAY 1 APRIL	4:00 pm 101 Science Hall

EVERYBODY WELCOME! Refreshments will be served at 3:30 p.m.

UNIVERSITY OF TEXAS ARLINGTON

Physics Department

Reminder: Special Project #5

- Prove that the wave function $\Psi=A[\sin(kx-\omega t)+i\cos(kx-\omega t)]$ is a good solution for the time-dependent Schrödinger wave equation. Do NOT use the exponential expression of the wave function. (10 points)
- Determine whether or not the wave function $\Psi=Ae^{-\alpha|x|}$ satisfy the time-dependent Schrödinger wave equation. (10 points)
- Due for this special project is Wednesday, Apr. 3.
- You MUST have your own answers!

Reminder: Special Project #6

- Derive the following using trigonometric identities

$$A\cos\left(k_1x-\omega_1t\right)+A\cos\left(k_2x-\omega_2t\right)=$$

$$2A\cos\left(\frac{k_1-k_2}{2}x-\frac{\omega_1-\omega_2}{2}t\right)\cos\left(\frac{k_1+k_2}{2}x-\frac{\omega_1+\omega_2}{2}t\right)=$$

- 10 points total for this derivation
- Due for this special project is Monday, Apr. 8.
- You MUST have your own answers!

Normalization and Probability

- The probability $P(x)\,dx$ of a particle being between x and $X + dx$ was given by the equation

$$P(x)dx = \Psi^*(x,t)\Psi(x,t)dx$$

- Here Ψ^* denotes the complex conjugate of Ψ
- The probability of the particle being between x_1 and x_2 is given by

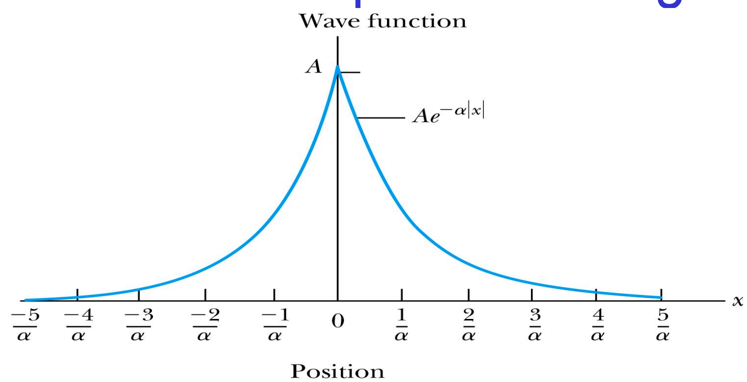
$$P = \int_{x_1}^{x_2} \Psi^* \Psi \, dx$$

- The wave function must also be normalized so that the probability of the particle being somewhere on the x axis is 1.

$$\int_{-\infty}^{+\infty} \Psi^*(x,t)\Psi(x,t)dx = 1$$

Ex 6.4: Normalization

Consider a wave packet formed by using the wave function that $Ae^{-\alpha|x|}$, where A is a constant to be determined by normalization. Normalize this wave function and find the probabilities of the particle being between 0 and $1/\alpha$, and between $1/\alpha$ and $2/\alpha$.



$$\Psi = Ae^{-\alpha|x|}$$

Probabilit y density

$$\int_{-\infty}^{+\infty} \Psi^* \Psi dx = \int_{-\infty}^{+\infty} \left(Ae^{-\alpha|x|}\right)^* \left(Ae^{-\alpha|x|}\right) dx = \int_{-\infty}^{+\infty} \left(A^* e^{-\alpha|x|}\right)\left(Ae^{-\alpha|x|}\right) dx =$$

$$= \int_{-\infty}^{+\infty} A^2 e^{-2\alpha|x|} dx = 2\int_{0}^{+\infty} A^2 e^{-2\alpha x} dx = \left.\frac{2A^2}{-2\alpha} e^{-2\alpha x}\right|_0^{+\infty} = 0 + \frac{A^2}{\alpha} = 1$$

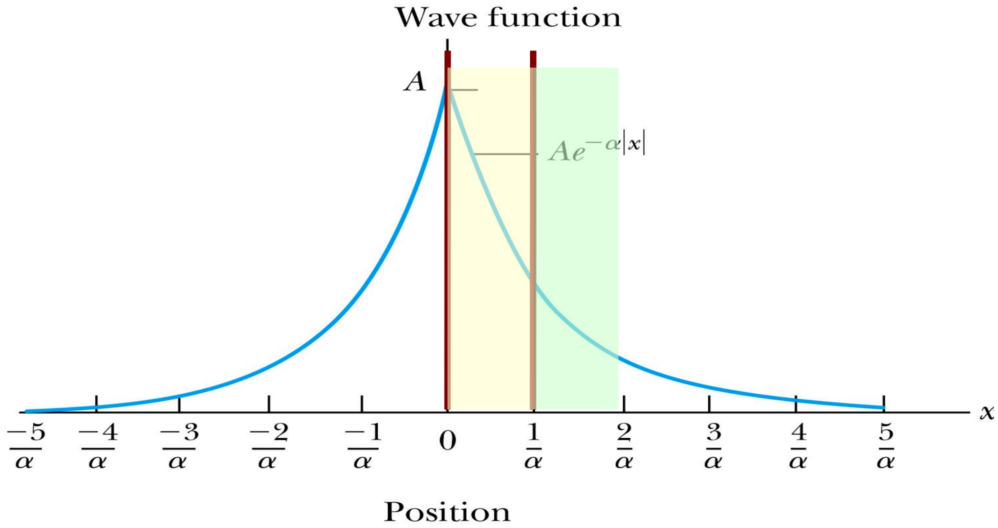
$$A = \sqrt{\alpha}$$

Normalized Wave Function

$$\Psi = \sqrt{\alpha}\, e^{-\alpha|x|}$$

Ex 6.4: Normalization, cont'd

Using the wave function, we can compute the probability for a particle to be with 0 to $1/\alpha$ and $1/\alpha$ to $2/\alpha$.



$$\Psi = \sqrt{\alpha}\, e^{-\alpha|x|}$$

For 0 to $1/\alpha$:

$$P = \int_0^{1/\alpha} \Psi^* \Psi dx = \int_0^{1/\alpha} \alpha e^{-2\alpha x} dx = \frac{\alpha}{-2\alpha} e^{-2\alpha x}\Big|_0^{1/\alpha} = -\frac{1}{2}\left(e^{-2} - 1\right) \approx 0.432$$

For $1/\alpha$ to $2/\alpha$:

$$P = \int_{1/\alpha}^{2/\alpha} \Psi^* \Psi dx = \int_{1/\alpha}^{2/\alpha} \alpha e^{-2\alpha x} dx = \frac{\alpha}{-2\alpha} e^{-2\alpha x}\Big|_{1/\alpha}^{2/\alpha} = -\frac{1}{2}\left(e^{-4} - e^{-2}\right) \approx 0.059$$

How about $2/\alpha$:to ∞?

Properties of a Valid Wave Function

Boundary conditions

1) To avoid infinite probabilities, the wave function must be **finite everywhere**.
2) To avoid multiple values of the probability, the wave function must be **single valued**.
3) For a **finite potential**, the wave function and its derivatives must be **continuous**. This is required because the second-order derivative term in the wave equation must be single valued. (There are exceptions to this rule when V is infinite.)
4) In order to normalize the wave functions, they must **approach zero as *x* approaches infinity**.

Solutions that do not satisfy these properties do not generally correspond to physically realizable circumstances.

Time-Independent Schrödinger Wave Equation

- The potential in many cases will not depend explicitly on time.
- The dependence on time and position can then be separated in the Schrödinger wave equation. Let, $\Psi(x,t)=\psi(x)f(t)$

which yields: $i\hbar\psi(x)\frac{\partial f(t)}{\partial t}=-\frac{\hbar^2 f(t)}{2m}\frac{\partial^2\psi(x)}{\partial x^2}+V(x)\psi(x)f(t)$

Now divide by the wave function: $i\hbar\frac{1}{f(t)}\frac{\partial f(t)}{\partial t}=-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2}+V(x)$

- The *left side* of this last equation depends only on time, and *the right side* depends only on spatial coordinates. Hence each side must be equal to a constant. The time dependent side is

$$i\hbar\frac{1}{f}\frac{df}{dt}=B$$

Time-Independent Schrödinger Wave Equation(con't)

- We integrate both sides and find: $i\hbar\int\frac{df}{f}=\int B\,dt \Rightarrow i\hbar\ln f = Bt + C$

  where *C* is an integration constant that we may choose to be 0. Therefore

$$\ln f = \frac{Bt}{i\hbar}$$

  This determines *f* to be $f(t)=e^{Bt/i\hbar}=e^{-iBt/\hbar}$. Comparing this to the time dependent portion of the free particle wave function $e^{-i\omega t}=e^{-iBt/\hbar}$

$$\Rightarrow B=\hbar\omega=E \qquad \Rightarrow \qquad i\hbar\frac{1}{f(t)}\frac{\partial f(t)}{\partial t}=E$$

- This is known as the **time-independent Schrödinger wave equation**, and it is a fundamental equation in quantum mechanics.

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

Stationary State

- Recalling the separation of variables: $\Psi(x,t)=\psi(x)f(t)$
  and with $f(t)=e^{-i\omega t}$ the wave function can be written as: $\Psi(x,t)=\psi(x)e^{-i\omega t}$
- The probability density becomes:

$$\Psi^*\Psi=\psi^2(x)\left(e^{i\omega t}e^{-i\omega t}\right)=\psi^2(x)$$

- The probability distributions are constant in time. This is a standing wave phenomena that is called the stationary state.

Comparison of Classical and Quantum Mechanics

- Newton's second law and Schrödinger's wave equation are both differential equations.
- Newton's second law can be derived from the Schrödinger wave equation, so the latter is the more fundamental.
- Classical mechanics only appears to be more precise because it deals with macroscopic phenomena. The underlying uncertainties in macroscopic measurements are just too small to be significant.

Expectation Values

- The **expectation value** is the expected result of the average of many measurements of a given quantity. The expectation value of *x* is denoted by <*x*>.
- Any measurable quantity for which we can calculate the expectation value is called the **physical observable**. The expectation values of physical observables (for example, position, linear momentum, angular momentum, and energy) **must be real**, because the experimental results of measurements are real.
- The average value of *x* is $$\bar{x} = \frac{N_1 x_1 + N_2 x_2 + N_3 x_3 + N_4 x_4 + \cdots}{N_1 + N_2 + N_3 + N_4 + \cdots} = \frac{\sum_i N_i x_i}{\sum_i N_i}$$

Continuous Expectation Values

- We can change from discrete to continuous variables by using the probability $P(x,t)$ of observing the particle at the particular x.

$$\bar{x} = \frac{\int_{-\infty}^{+\infty} xP(x)\,dx}{\int_{-\infty}^{+\infty} P(x)\,dx}$$

- Using the wave function, the expectation value is:

$$\bar{x} = \frac{\int_{-\infty}^{+\infty} x\Psi(x,t)^{*}\Psi(x,t)\,dx}{\int_{-\infty}^{+\infty} \Psi(x,t)^{*}\Psi(x,t)\,dx}$$

- The expectation value of any function $g(x)$ for a normalized wave function:

$$\langle g(x)\rangle = \int_{-\infty}^{+\infty} \Psi(x,t)^{*} g(x)\Psi(x,t)\,dx$$

Momentum Operator

- To find the expectation value of *p*, we first need to represent *p* in terms of *x* and *t*. Consider the derivative of the wave function of a free particle with respect to *x*:

$$\frac{\partial\Psi}{\partial x} = \frac{\partial}{\partial x}\left[e^{i(kx-\omega t)}\right] = ike^{i(kx-\omega t)} = ik\Psi$$

With $k = p/\hbar$ we have $\dfrac{\partial\Psi}{\partial x} = i\dfrac{p}{\hbar}\Psi$

This yields $$p\left[\Psi(x,t)\right] = -i\hbar\frac{\partial\Psi(x,t)}{\partial x}$$

- This suggests we define the momentum operator as $\hat{p} = -i\hbar\dfrac{\partial}{\partial x}$
- The expectation value of the momentum is

$$\langle p\rangle = \int_{-\infty}^{+\infty}\Psi^*(x,t)\hat{p}\Psi(x,t)\,dx = -i\hbar\int_{-\infty}^{+\infty}\Psi^*(x,t)\frac{\partial\Psi(x,t)}{\partial x}dx$$

Position and Energy Operators

- The position x is its own operator as seen above.
- The time derivative of the free-particle wave function is

$$\frac{\partial \Psi}{\partial t} = \frac{\partial}{\partial t}\left[e^{i(kx-\omega t)}\right] = -i\omega e^{i(kx-\omega t)} = -i\omega\Psi$$

Substituting $\omega = E/\hbar$ yields $E\left[\Psi(x,t)\right] = i\hbar\frac{\partial \Psi(x,t)}{\partial t}$

- So the energy operator is $\hat{E} = i\hbar\frac{\partial}{\partial t}$
- The expectation value of the energy is

$$\langle E\rangle = \int_{-\infty}^{+\infty}\Psi^*(x,t)\hat{E}\Psi(x,t)\,dx = i\hbar\int_{-\infty}^{+\infty}\Psi^*(x,t)\frac{\partial \Psi(x,t)}{\partial t}dx$$