2D Course Review: Fall 2003

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10 Important New Ideas You Learnt In This Course

1. Special Theory of Relativity
    1. Simultaneity : Time is not an absolute quantity
    2. Space-time, mass-energy
    3. Lorentz Transformation between Frames of References
        1. Length, time, velocity, momentum and force
2. Particle Nature of EM Waves
    1. Blackbody radiation and Ultraviolet Catastrophe
    2. Energy Quantization ….Planck's constant
        1. Photoelectric effect
        2. Compton effect

3. Wave Nature of Matter
    1. De Broglie and Matter Waves → Davisson-Germer Experiment
    2. Wave Packets model of particles:
    3. Heisenberg's Uncertainty Principle !!
        1. How to break nature's laws of conservation and still not go to jail
            1. Energy Conservation
            2. Momentum Conservation
        2. Quantum Tunneling across barriers : The great Escape !

10 Important New Ideas You Learnt In This Course

4. Wave-Particle Duality &Correspondence principle as $n \rightarrow \infty$
5. Statistical Nature of description for Subatomic Particles
6. Rules of Quantum Mechanics for Subatomic systems
7. Schrodinger Equation For particles Under a Potential:
   - Time dependent and Time independent S. Eqn.
   - Wave Function and Probabilities
   - Operators and Expectation values
   - How to propagate the wavefunction $\Psi(x,t=0)$ in time
8. Free particles and Trapped systems
   - Spectrum of energies for trapped systems
     - Particle in a box
     - Harmonic Oscillator
     - Hydrogen atom and explanation of Spectroscopic data
9. Degenerate Systems and how to break Energy Degeneracy
10. Principle of superposition & Designer Wave functions!
    - Spatially characteristic electron clouds !

Relativity !

The two basic postulates of the **special theory of relativity** are as follows:

- The laws of physics must be the same for all observers moving at constant velocity with respect to one another.
- The speed of light must be the same for all inertial observers, independent of their relative motion.

To satisfy these postulates, the Galilean transformations must be replaced by the **Lorentz transformations** given by

$$x' = \gamma(x - vt) \tag{1.25}$$

$$y' = y \tag{1.26}$$

$$z' = z \tag{1.27}$$

$$t' = \gamma\left(t - \frac{v}{c^2}x\right) \tag{1.28}$$

where

$$\gamma = \frac{1}{\sqrt{1 - (v^2/c^2)}} \tag{1.29}$$

In these equations, it is assumed that the primed system moves with a speed v along the xx' axes.

The relativistic form of the **velocity transformation** is

$$u'_x = \frac{u_x - v}{1 - (u_x v / c^2)} \tag{1.32}$$

where u_x is the speed of an object as measured in the S frame and u'_x is its speed measured in the S′ frame.

Some of the consequences of the special theory of relativity are as follows:

- Clocks in motion relative to an observer appear to be slowed down by a factor γ. This is known as **time dilation.**
- Lengths of objects in motion appear to be contracted in the direction of motion by a factor of $1/\gamma$. This is known as **length contraction.**
- Events that are simultaneous for one observer are not simultaneous for another observer in motion relative to the first.

These three statements can be summarized by saying that duration, length, and simultaneity are not absolute concepts in relativity.

The relativistic expression for the **momentum** of a particle moving with a velocity **u** is

$$\mathbf{p} \equiv \frac{m\mathbf{u}}{\sqrt{1-(u^2/c^2)}} = \gamma m\mathbf{u} \tag{1.35}$$

where γ is redefined in the following equation as

$$\gamma = \frac{1}{\sqrt{1-(u^2/c^2)}}$$

The relativistic expression for the **kinetic energy** of a particle is

$$K = \gamma mc^2 - mc^2 \tag{1.42}$$

where mc^2 is called the **rest energy** of the particle.

The total energy E of a particle is related to the mass through the expression:

$$E = \gamma mc^2 = \frac{mc^2}{\sqrt{1-(u^2/c^2)}} \tag{1.44}$$

Another useful expression relates the relativistic momentum to the total energy through the equation

$$E^2 = p^2c^2 + (mc^2)^2 \tag{1.45}$$

Finally, the law of the conservation of mass and energy states that the sum of the masses and energies of a system of particles before interaction must equal the sum of the masses and the energies of the particles after interaction where the energy of the *i*th particle is

$$E = \frac{m_i c^2}{\sqrt{1 - (u_i^2 / c^2)}}$$

Application of the conservation of mass and energy to the specific cases of (1) the fission of a heavy nucleus at rest and (2) the fusion of several particles into a composite nucleus with less total mass allows us to define (1) the energy released per fission, Q, and (2) the binding energy of a composite system, *BE*.

Aftermath of BlackBody Radiation and Ultraviolet Catastrophe

Planck quantized the energy of atomic oscillators, but Einstein extended the concept of quantization to light itself. In Einstein's view, light of frequency f consists of a stream of particles, called *photons*, each with energy $E = hf$. The photoelectric effect, a process in which electrons are ejected from a metallic surface when light of sufficiently high frequency is incident on the surface, can be simply explained with the photon theory. According to this theory, the maximum kinetic energy of the ejected photoelectron, K_{max}, is given by

$$K_{\text{max}} = hf - \phi \tag{2.23}$$

where ϕ is the work function of the metal.

Compton Scattering and Particle Nature of Light

Although the idea that light consists of a stream of photons with energy hf was put forward in 1905, the idea that these photons also carry momentum was not experimentally confirmed until 1923. In that year it was found that x-rays scattered from free electrons suffer a simple shift in wavelength with scattering angle, known as the Compton shift. When an x-ray of frequency f is viewed as a *particle* with *energy* hf and *momentum* hf/c, x-ray–electron scattering can be correctly analyzed to yield the Compton shift formula:

$$\Delta\lambda = \frac{h}{m_e c}(1 - \cos\theta) \tag{2.28}$$

Here m_e is the mass of the electron, and θ is the x-ray scattering angle.

The striking success of the photon theory in explaining interactions between light and electrons contrasts sharply with the success of classical wave theory in explaining the polarization, reflection, and interference of light. This leaves us with the dilemma of whether light is a wave or a particle. The currently accepted view suggests that light has both wave and particle characteristics, and that these characteristics together constitute a complementary view of light.

Inside an Atom: Rutherford Thru Bohr

- **Rutherford's scattering of α particles from gold atoms**, which established the nuclear model of the atom. By measuring the rate of scattering of α particles into an angle ϕ, Rutherford was able to establish that most of the mass and all of the positive charge of an atom, $+Ze$, are concentrated in a minute volume of the atom with a radius of about 10^{-14} m.

The explanation of the motion of electrons within the atom and of the rich and elaborate series of spectral lines emitted by the atom was given by Bohr. Bohr's theory was based partly on classical mechanics and partly on some startling new quantum ideas. **Bohr's postulates** were:

- Electrons move about the nucleus in circular orbits determined by Coulomb's and Newton's laws.
- Only certain orbits are stable. The electron does not radiate electromagnetic energy in these special orbits, and because the energy is constant with time these are called *stationary states.*
- A spectral line of frequency f is emitted when an electron jumps from an initial orbit of energy E_i to a final orbit of energy E_f, where

$$hf = E_i - E_f \tag{3.23}$$

- The sizes of the stable electron orbits are determined by requiring the electron's angular momentum to be an integral multiple of $\hbar$:

$$m_e vr = n\hbar \qquad n = 1, 2, 3, \ldots \tag{3.24}$$

These postulates lead to quantized orbits and quantized energies for a single electron orbiting a nucleus with charge $+Ze$, given by

$$r_n = \frac{n^2 a_0}{Z} \tag{3.35}$$

Matter Waves !

Every lump of matter of mass m and momentum p has wavelike properties with wavelength given by the de Broglie relation

$$\lambda = \frac{h}{p} \tag{4.1}$$

By applying this wave theory of matter to electrons in atoms, de Broglie was able to explain the appearance of integers in certain Bohr orbits as a natural consequence of electron wave interference. In 1927, Davisson and Germer demonstrated directly the wave nature of electrons by showing that low-energy electrons were diffracted by single crystals of nickel. In addition, they confirmed Equation 4.1.

Uncertainty Principles of Quantum Behavior !

for position and momentum:

$$\Delta p_x \, \Delta x \geqslant \frac{\hbar}{2} \tag{4.31}$$

In a similar fashion one can show that an energy–time uncertainty relation exists given by

$$\Delta E \, \Delta t \geqslant \frac{\hbar}{2} \tag{4.34}$$

Statistical Nature of Quantum Behavior and Ψ

In quantum mechanics matter waves are represented by a wavefunction $\Psi(x, y, z, t)$. The probability of finding a particle represented by Ψ in a small volume centered at (x, y, z) at time t is proportional to $|\Psi|^2$. The wave–particle duality of electrons may be seen by considering the passage of electrons through two narrow slits and their arrival at a viewing screen. We find that although the electrons are detected as particles at a localized spot on the screen, the probability of arrival at that spot is determined by finding the intensity of two interfering matter waves.

Wave Functions and What they Tell You

In quantum mechanics, matter waves (or de Broglie waves) are represented by a wavefunction $\Psi(x, t)$. The probability that a particle constrained to move along the x axis will be found in an interval dx at time t is given by $|\Psi|^2\, dx$. These probabilities summed over all values of x must total 1 (certainty). That is,

$$\int_{-\infty}^{\infty} |\Psi|^2\, dx = 1 \tag{5.2}$$

This is called the **normalization condition.** Furthermore, the probability that the particle will be found in any interval $a \leqslant x \leqslant b$ is obtained by integrating the **probability density** $|\Psi|^2$ over this interval.

Aside from furnishing probabilities, the wavefunction can be used to find the average, or **expectation value,** of any dynamical quantity. The average position of a particle at any time t is

$$\langle x \rangle = \int_{-\infty}^{\infty} \Psi^* x \Psi\, dx \tag{5.31}$$

In general, the average value of any observable Q at time t is

$$\langle Q \rangle = \int_{-\infty}^{\infty} \Psi^*[Q]\Psi \, dx \tag{5.37}$$

where $[Q]$ is the associated operator. The operator for position is just $[x] = x$, and that for particle momentum is $[p] = (\hbar/i)\partial/\partial x$.

The wavefunction Ψ must satisfy the **Schrödinger equation**

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + U(x)\Psi(x, t) = i\hbar\frac{\partial\Psi}{\partial t} \tag{5.10}$$

Separable solutions to this equation, called **stationary states**, are $\Psi(x, t) = \psi(x)e^{-i\omega t}$, with $\psi(x)$ a time-independent wavefunction satisfying the **time-independent Schrödinger equation**

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U(x)\psi(x) = E\psi(x) \tag{5.13}$$

The approach of quantum mechanics is to solve Equation 5.13 for ψ and E, given the potential energy $U(x)$ for the system. In doing so, we must require

- that $\psi(x)$ be continuous,
- that $\psi(x)$ be finite for all x including $x = \pm\infty$,
- that $\psi(x)$ be single-valued, and
- that $d\psi/dx$ be continuous wherever $U(x)$ is finite.

Quantum Mechanics in 3 Dimensions

In three dimensions, the matter wave intensity $|\Psi(\mathbf{r}, t)|^2$ represents the probability per unit volume for finding the particle at $\mathbf{r}$ at time t. Probabilities are found by integrating this probability density over the volume of interest.

The wavefunction itself must satisfy the Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + U(r)\Psi = i\hbar\frac{\partial\Psi}{\partial t} \tag{7.1}$$

Stationary states are solutions to this equation in separable form: $\Psi(\mathbf{r}, t) = \psi(\mathbf{r})e^{-i\omega t}$ with $\psi(\mathbf{r})$ satisfying

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + U(r)\psi(\mathbf{r}) = E\psi(\mathbf{r}) \tag{7.5}$$

This is the *time-independent Schrödinger equation*, from which we obtain the time-independent wavefunction $\psi(\mathbf{r})$ and the allowed values of particle energy E.

Particle in a 3D Box or Well with Rigid Walls
Concept of Degeneracy for a Cube

For a particle confined to a cubic box whose sides are L, the magnitudes of the components of particle momentum normal to the walls of the box can be made sharp, as can the particle energy. The sharp momentum values are quantized as

$$|p_x| = n_1 \frac{\pi\hbar}{L}$$

$$|p_y| = n_2 \frac{\pi\hbar}{L} \qquad (7.8)$$

$$|p_z| = n_3 \frac{\pi\hbar}{L}$$

and the allowed energies are found to be

$$E = \frac{\pi^2\hbar^2}{2mL^2}\{n_1{}^2 + n_2{}^2 + n_3{}^2\} \qquad (7.9)$$

Hydrogen Atom : Trapped in a Coulomb Force

For particles acted on by a *central force*, the *angular momentum* **L** is a constant of the classical motion and is quantized along with particle energy. Wavefunctions for which the z component L_z and magnitude $|\mathbf{L}|$ of angular momentum are simultaneously sharp are the *spherical harmonics* $Y_\ell^{m_\ell}(\theta, \phi)$ in the spherical coordinate angles θ and ϕ. For any central force, angular momentum is quantized by the rules

$$|\mathbf{L}| = \sqrt{\ell(\ell + 1)}\,\hbar$$

and

$$L_z = m_\ell \hbar \tag{7.14}$$

The *orbital quantum number* ℓ must be a nonnegative integer. For a fixed value of ℓ, the *magnetic quantum number* m_ℓ is restricted to integer values lying between $-\ell$ and $+\ell$. Since $|\mathbf{L}|$ and L_z are quantized differently, the classical freedom to orient the z axis in the direction of **L** must be abandoned. This stunning conclusion is the essence of *space quantization*. Furthermore, no two components of **L**, such as L_z and L_y, can be sharp simultaneously. This implies a lower limit to the uncertainty product $\Delta L_z \Delta L_y$ and gives rise to an uncertainty principle for the components of angular momentum.

A central force of considerable importance is the force on the electron in a one-electron atom or ion. This is the *Coulomb* force, described by the potential energy $U(r) = -kZe^2/r$, where Z is the atomic number of the nucleus. The allowed energies for this case are given by

$$E_n = -\frac{ke^2}{2a_0}\left\{\frac{Z^2}{n^2}\right\} \qquad n = 1, 2, \ldots \tag{7.38}$$

This coincides exactly with the results obtained from the Bohr theory. The energy depends only on the *principal quantum number n*. For a fixed value of n, the orbital and magnetic quantum numbers are restricted as

$$\ell = 0, 1, 2, \ldots, n-1$$

$$m_\ell = 0, \pm 1, \pm 2, \ldots, \pm \ell \tag{7.39}$$

All states with the same principal quantum number n form a *shell*, identified by the letters $K, L, M, \ldots$ (corresponding to $n = 1, 2, 3, \ldots$). All states with the same values of n and ℓ form a *subshell*, designated by the letters $s, p, d, f, \ldots$ (corresponding to $\ell = 0, 1, 2, \ldots$).

The wavefunctions for an electron in hydrogen or a hydrogen-like ion

$$\psi(r, \theta, \phi) = R_{n,\ell}(r)\, Y_\ell^{m_\ell}(\theta, \phi)$$

The Hydrogen like Atom : One electron around a Nucleus

The wavefunctions for an electron in hydrogen or a hydrogen-like ion

$$\psi(r, \theta, \phi) = R_{n,\ell}(r) Y_{\ell}^{m_\ell}(\theta, \phi)$$

depend on the three quantum numbers n, ℓ, and m_ℓ, and are products of spherical harmonics multiplied by radial wavefunctions $R_{n,\ell}(r)$. The *pseudo-wavefunction* $g(r) = rR_{n,\ell}(r)$ is analogous to the wavefunction $\psi(x)$ in one dimension; the intensity of $g(r)$ gives the *radial probability density*

$$P(r) = |g(r)|^2 = r^2 |R_{n,\ell}(r)|^2 \tag{7.44}$$

$P(r)\, dr$ is the probability that the electron will be found at a distance between r and $r + dr$ from the nucleus. The *most probable distance* is the one that maximizes $P(r)$ and generally differs from the *average distance* $\langle r \rangle$ calculated as

$$\langle r \rangle = \int_0^\infty rP(r)\, dr \tag{7.46}$$

The most probable values are found to coincide with the radii of the allowed orbits in the Bohr theory.