Quantum Mechanics and Atomic Physics


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Heisenberg Uncertainty Principle

- Werner Heisenberg (1927) *Gadenken* (thought) experiments.
- Single-slit diffraction of electrons, of wavelength $\lambda$
- $w =$ slit spacing
- Diffraction first minimum $\theta$ at $(w \sin \theta = \lambda)$
- Uncertainty in position $\Delta x = w$
- Uncertainty in $p_x \approx$ momentum needed to send electron to first minimum.

So $\Delta p_x \geq p \cdot \sin \theta = \left( \frac{h}{\lambda} \right) \left( \frac{\lambda}{w} \right) = \frac{h}{w} = \frac{h}{\Delta x}$

$\Rightarrow \Delta p_x \cdot \Delta x \geq h$

More sophisticated analysis:

$\Delta p_x \cdot \Delta x \geq \frac{h}{4\pi}$

Define : $\tilde{h} = \frac{h}{2\pi}$ then $\Delta p_x \cdot \Delta x \geq \frac{\tilde{h}}{2}$

Protons and neutrons in nuclei have minimum kinetic energies of a few MeV. So nuclear binding energies have to exceed few MeV.
Example

In an atomic nucleus, a proton is confined to $\Delta x \approx 10^{-15} \text{m}$. Find its minimum kinetic energy. ($m_p = 938 \text{MeV}/c^2$)

$$\Delta p_x \geq \frac{\hbar}{\Delta x} = 100 \frac{\text{MeV}}{c} \text{ for } \Delta x = 10^{-15} \text{m}$$

So, $P_{\text{min}} \approx 100 \frac{\text{MeV}}{c}$

So, $E_{\text{min}} = \sqrt{(100)^2 + (938)^2}$

$= 943 \text{MeV}$

So, $K_{\text{min}} = E_{\text{min}} - E_0 = 943 - 938 = 5 \text{MeV}$

So nuclear binding energies must be at least 5 MeV! Recall hydrogen atom’s binding energy is 13.6 eV.
Example, con’t

Now suppose there were electrons in nuclei...

\[ \Delta p_x \geq \frac{100 \text{ MeV}}{c} \text{ as above} \]

\[ P_{\text{min}} = \frac{100 \text{ MeV}}{c} \text{ as above} \]

\[ \text{But} \quad E_{\text{min}} = \sqrt{(100)^2 + (0.511)^2} \approx 100 \text{ MeV} \]

\[ \text{and} \quad k_{\text{min}} = E_{\text{min}} - E_0 = 100 - 0.511 \approx 100 \text{ MeV} \]
Another Form of Uncertainty Principle

- Measure frequency of de Broglie waves: count how many pass in time $\Delta t$.

\[
\nu = \frac{\# \text{waves}}{\Delta t} \quad \text{but } \Delta(\# \text{waves}) \geq 1
\]

So $\Delta \nu \geq \frac{1}{\Delta t} \Rightarrow \Delta \nu \Delta t \geq 1$

Also $E = h\nu \Rightarrow \Delta E = h\Delta \nu \Rightarrow \Delta \nu = \frac{\Delta E}{h}$

So $\frac{\Delta E}{h} \cdot \Delta t \geq 1 \Rightarrow \Delta E \cdot \Delta t \geq \frac{\hbar}{2}$

- Objects of finite lifetime cannot have a fixed rest mass.

- Particles such as baryon and meson resonances may have lifetimes of $10^{-23} \text{ s} \Rightarrow \Delta E \geq 30\text{MeV}$ (see next Example)

- The act of measurement or observation necessarily disturbs the system being observed.
Example

- Objects of finite lifetime don’t have a fixed value of mass! There exist particles of lifetime $\sim 10^{-23}$s. What is their uncertainty in mass?

\[
\Delta E \geq \frac{\hbar}{2\Delta t} = \frac{6.63 \times 10^{-34} \text{ J-s}}{4\pi \times 10^{-23} \text{s}} \times \frac{1 \text{ eV}}{1.6 \times 10^{-19} \text{ J}} \times \frac{1 \text{ MeV}}{10^6 \text{ eV}}
\]

\[
= 33 \text{ MeV}
\]

$\sim 33 \text{ MeV}$

M (MeV/c²)
Let’s recap what we know so far

- We’ve seen experimental (and theoretical) evidence that shows that particles of microscopic systems move according to some form of wave motion.
- Aspects of a microscopic particle acts as if certain aspects of its behavior are governed by de Broglie’s postulate of a wave or “wavefunction”.
- How this “wavefunction” affects our description of the particle and its behavior is the subject of quantum mechanics (or wave mechanics).
- This was developed by Erwin Schrodinger, Heisenberg and others from 1925-26.
- Let’s first look at the classical model of a wave....
Classical vs. Quantum Physics

Classical physics: \( m \frac{d^2 \vec{r}}{dt^2} = \vec{F}(\vec{r}, t) \)

In principle, if we know \( \vec{F}(\vec{r}, t) \) exactly, we could solve for \( \vec{r}(t) \) and get a precise answer.

Quantum Physics: It is **not** possible, not even in principle, not even if we know \( \vec{F}(\vec{r}, t) \) exactly.

- But: Quantum mechanics gives us a way to calculate the probability of each possible outcome of a measurement.
- Consider a particle of mass \( m \) and suppose the force on it is \( F(x,t) \)
- Then the potential energy is:

\[
V(x,t) = -\int F(x,t) \, dx
\]
The Classical Wave Equation

- **Traveling wave on a string is described by a “wave function”:** \( y = f(x,t) \)

- **Harmonic wave:**
  \[
  y = A \cos \left( \frac{2\pi}{\lambda} (x - vt) \right)
  \]
  
  \( A = \text{Amplitude}, \ \lambda = \text{wavelength}, \ v = \text{wave speed} \)

  Speed of string molecules is \( \frac{dy}{dt} \)

  \[
  y = A \cos \left( \frac{2\pi}{\lambda} x - 2\pi vt \right) = A \cos (kx - \omega t)
  \]

  Wave number \( k = \frac{2\pi}{\lambda} \), Angular frequency \( \omega = 2\pi v \)

(Used \( \lambda \cdot v = v \))
The Classical Wave Equation, con’t

- Can we express this more generally?
- Such generalized expressions of physical laws take the form of partial differential equations:

\[
\begin{align*}
\text{In general:} \\
y &= f(x-ht) = f(z) \\
\text{where} \\
z &= x-ht \\
\frac{\partial y}{\partial x} &= \frac{\partial^2 y}{\partial z^2} - \frac{h}{c} \frac{\partial y}{\partial z} \\
\frac{\partial y}{\partial t} &= -\frac{h}{c} \frac{\partial y}{\partial z}
\end{align*}
\]
We can then form an identity:

\( \frac{\partial y}{\partial t} + \nu \frac{\partial y}{\partial x} = -\nu \frac{\partial y}{\partial z} + \nu \frac{\partial^2 y}{\partial x^2} = 0 \)

Then,

\( \frac{\partial}{\partial t} \left( \frac{\partial y}{\partial t} + \nu \frac{\partial y}{\partial x} \right) = \frac{\partial^2}{\partial t^2} \left( \frac{\partial y}{\partial t} + \nu \frac{\partial y}{\partial x} \right) = 0 \)

\( \frac{\partial^2 y}{\partial t^2} + \nu \frac{\partial}{\partial x} \left( \frac{\partial y}{\partial t} + \nu \frac{\partial y}{\partial x} \right) = 0 \)

\( \frac{\partial^2 y}{\partial t^2} = -\nu \frac{\partial^2 y}{\partial x^2} \)

\[ \boxed{\frac{\partial^2 y}{\partial t^2} = \nu^2 \frac{\partial^2 y}{\partial x^2}} \]  

Classical Wave Equation
Wavefunction $\Psi$

- **Free particle $\rightarrow$ de Broglie wave $\rightarrow$ Wavefunction**

- $\Psi(x,t)$ is a general complex number:
  
  $\Psi = A + iB$ or $\text{Re}^i\theta$ where $i=\sqrt{-1}$.

- **Probability of finding particle between $x$ and $(x+dx)$ at time $t$ is:**
  
  $P(x,t)dx = \Psi^*(x,t) \Psi(x,t)dx$

  where $\Psi^*(x,t)$ is the complex conjugate of $\Psi$

  $P(x,t) = \Psi^*(x,t) \Psi(x,t) = (A-iB)(A+iB) = A^2 - i^2B^2 = A^2 + B^2$

  So $P(x,t)$ is real and positive .... Whew!
Free Particle

- A free particle is one subject to no force.
- Reasonable assumptions concerning the properties of desired quantum mechanical wave equation:

1. It must be consistent with postulates of de Broglie and Einstein: \( \lambda = h/p \) and \( \nu = E/h \)
2. It must be consistent with energy equation: \( E = p^2/2m + V \)
3. It must be linear. (see next slide)
4. Forces of interest are derivable from potentials: \( F = -\partial V(x,t)/\partial x \)
Linearity

- If $\Psi_1(x,t)$ and $\Psi_2(x,t)$ are two different solutions to the equation for a given potential energy $V$, then any arbitrary linear combination of these solutions, $\Psi(x,t) = c_1 \Psi_1(x,t) + c_2 \Psi_2(x,t)$, is also a solution.
- It involves the first (linear) power of $\Psi_1(x,t)$ and $\Psi_2(x,t)$
- $c_1$ and $c_2$ can have any (arbitrary) complex values
- Linearity ensures we can add together wave functions
  - Constructive and destructive interference
  - Principle of superposition
Free Particle

- For a free particle \( F=0 \)
- So \( F=-\frac{\partial V(x,t)}{\partial x}=0 \) if \( V \) = constant
- Linear momentum \( p \) will be constant and therefore its total energy will be constant

Let’s make the connection from the classical wave to quantum mechanical matter waves by using the classical sinusoidal wavefunction as an example:

\[
y = A \cos \frac{2\pi}{\lambda} (x - vt)
\]

And let’s assume no time dependence.
This IS the non-relativistic, 1-Dimensional, time-independent Schrodinger equation! (S.E.)
Time-Independent S.E. in 3-D

Now the wavefunction is $\Psi(r)$:

$$\frac{-\hbar^2}{2m} \nabla^2 \psi(r) + V(r) \psi(r) = E \psi(r)$$

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

Laplacian operator

In 3-D dimensions.
We just derived Schrödinger’s equation!

- There are three things to note in what we did:
  1. The classical wave equation was NOT used - we used only a prototype wavefunction
  2. We did not use the concept of quantization
  3. The total energy $E$ appears explicitly in the resulting differential equation
     - This is unusual from the point of view of classical physics. For example, Newton’s law $F=ma$ makes no mention of energy.

- Schrödinger’s equation is an “eigenvalue equation”:
  - We will see later that for a given value of $V$ and a set of “boundary conditions” there will be a restricted set of functions $\Psi(x,t)$ satisfying the equation, and each of these corresponds to a particular value of $E$
  - The quantized energy states!
Let’s try to include time-dependence

\[ \psi = A \cos \frac{2\pi}{\hbar} (x - vt) \]

\[ \omega = 2\pi \nu = 2\pi \frac{E}{h} = \frac{E}{h} \]

\[ \Psi = A \cos \left( \frac{t}{\hbar} (p x - E t) \right) \]

\[ \frac{\partial \psi}{\partial t} = \frac{E}{\hbar} A \sin (\cdots) \]

\[ \Rightarrow \quad A^2 \sin^2 (\cdots) + A^2 \cos^2 (\cdots) = A^2 \]

\[ A \sin (\cdots) = \pm \sqrt{A^2 - A^2 \cos^2 (\cdots)} \]

\[ = \pm \sqrt{A^2 - \psi^2} \]

\[ \Rightarrow \quad \frac{\partial \psi}{\partial t} = \pm \frac{E}{\hbar} \sqrt{A^2 - \psi^2} \]

\[ E = \frac{i \hbar}{\sqrt{A^2 - \psi^2}} \quad \frac{\partial \psi}{\partial t} \]

Insert into time-independent S.E.:

\[ -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x, t) \psi = \frac{i \hbar \psi}{\sqrt{A^2 - \psi^2}} \frac{\partial \psi}{\partial t} \]
Problems with this result?

- Let’s continue and discuss this next time.
Summary/Announcements

- We “derived” Schrödinger’s equation!
- Next time:
  - Schrödinger’s Equation continued
  - Probabilities and boundary conditions

- Recall, there is a copy of textbook(s) on reserve in the MSLC

- Next week:
  - Mon Sept 16:
    - First homework due