Quantum Mechanics and Atomic Physics Lecture 3: Schroedinger's Equation: Part I

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Announcement

- First homework due on Wednesday Sept 14 at the beginning of class: late homework will be accepted only until noon of the following day in my mail box with penalty of 20% deduction and the second HW will be due on Monday Sept 19!
- The text book is on reserve in SERC reading room

Let's recap

- We've seen experimental (and theoretical) evidence that shows that particles of microscopic systems move according to some form of wave motion.
- 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 $\underline{Classical physics}: m \frac{d^2 \vec{r}}{dt^2} = \vec{F}(\vec{r}, t)$

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:

$$V(x,t) = -\int F(x,t)dx$$

Schroedinger Equation

- Schroedinger equation for quantum mechanics is equivalent to Newton's equation for classical mechanics, that is: $m\frac{d^2\vec{r}}{dt^2} = \vec{F}(\vec{r},t)$.
- Schroedinger equation looks like:

 $-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r},t) + V(\vec{r},t)\psi(\vec{r},t) = i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t}$. If there is no time dependence, it reduces to: \hbar^2

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

which is called time-independent Schroedinger equation.

The Classical Wave Equation

- Traveling wave on a string is described by a "wave function" : y = f(x,t)
- Harmonic wave:

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

A = Amplitude, $\lambda =$ wavelength, v = wave speed

Speed of string molecules is $\frac{dy}{dt}$

$$y = A\cos(\frac{2\pi}{\lambda}x - 2\pi\nu t) = A\cos(kx - \omega t)$$

Wave number $k = \frac{2\pi}{\lambda}$, Angular frequency $\omega = 2\pi v$, where v is frequency not speed.



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:

Generally, wave is a function of both position and time. If we call the displacement of the wave propagating medium at position "x" and time "t" by "y", then y = f(x,t). However all wave functions can be expressed as y = f(x,t) = f(x-vt)

Classical wave Equation cont'

With z = x - vt, y = f(x - vt) = f(z). Remember, for $f(q(\alpha, \beta, \gamma))$, $\Im f = \Im f \Im g$, $\Im f = \Im f \Im g$, $\Im f \Im g \Im g$, $\Im \chi = \Im g \Im \chi$, $\Im g = \Im g \Im \beta$, $\Im \gamma \Im g \Im \gamma$ $\frac{\partial y}{\partial x} = \frac{\partial y}{\partial z} \frac{\partial z}{\partial x} = \frac{\partial y}{\partial z} \int \frac{\partial y}{\partial z} = \frac{\partial y}{\partial z} \int \frac{\partial y}{\partial x} = \frac{\partial y}{\partial z} \int \frac{\partial y}{\partial z} = \frac{\partial y}{\partial z} \int \frac{\partial y}{\partial z} = -\sqrt{\frac{\partial y}{\partial z}}$

Classical wave Equation cont'



Properties of Wave functions

Linearity

If $y_1, y_2, ..., y_n$ are solutions of the same wave equation, then any linear sum of them is also a solution of the wave equation; that is, a function of the form $y = a_1 y_1 + a_2 y_2 + ... + a_n y_n$ is also a solution.

Example

Which of the following are acceptable classical wave functions?
1. y = sin(x+vt)

2.
$$y = (\sin(x - vt))^2$$

3. $y = \cos[(x - vt)(x + vt)]$
4. $y = \exp(x + vt)^{3/4}$
5. $y = x\sin(x - vt)$
6. $y = \sin(x - vt) + 4\cos(x + vt)$
7. $y = \exp(x - vt)^{3/4} + 2\cos(x + vt)$
8. $y = \sin(x - vt)\cos(x + vt)$
9. $y = t\sin(x - vt)$

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.
 - 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 $F = -\partial V(x,t) / \partial x = 0$ 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.

Time-Independent S.E.

$$E = \frac{p^{2}}{am} + V, \quad \lambda = h/p$$

$$y = A \cos \frac{2\pi}{\lambda} (x - \nu t)$$

Let's extract p from y:

$$\frac{dy}{dx} = -A \lim_{X} \sin 2\pi (x - \nu t)$$

$$\frac{d^2 y}{dx^2} = -A\left(\frac{2\pi}{\lambda}\right)^2 \cos \frac{2\pi}{\lambda} (x - vt)$$
$$= -\left(\frac{2\pi}{\lambda}\right)^2 y = -\left(\frac{2\pi}{\lambda}\right)^2 y \qquad \pi = \frac{h}{2\pi}$$
$$= -\left(\frac{p}{\pi}\right)^2 y$$

$$P^{2} = -\frac{\hbar^{2}}{y} \frac{d^{2}y}{dx^{2}}$$

$$\Rightarrow E = -\frac{\hbar^{2}}{y} \frac{d^{2}y}{dx^{2}} + V$$

$$\boxed{-\frac{\hbar^{2}}{2m} \frac{d^{2}y}{dx^{2}} + V \cdot y} = E \cdot y$$

This IS the non-relativistic, 1-Dimensional, time-independent Schrodinger equation! (S.E.)

Time-Independent S.E. in 3-D

Now the wavefunction is $\Psi(\mathbf{r})$:

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

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \qquad \text{Laplacian} \\ \text{Operator} \\ \text{In } 3 - \text{Dimensions.}$$

We just derived Schrodinger'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.
- Schrodinger'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
 Ψ(x,t) satisfying the equation, and each of these corresponds to a particular value of E
 - The quantized energy states!

Example Problem

Problem 2-3 in your book

The Schrödinger equation is not the only possible "differential wave equation" consistent with the law of conservation of energy and the prototype waveform (2.2.5). "Derive" one other.

For simplicity let's assume two

$$\Psi(x) = A e^{\frac{i\rho x}{h}}$$

 $\frac{\partial \Psi}{\partial x} = (\frac{i\rho}{h})\Psi \implies P = -\frac{ih}{\Psi} \frac{d\Psi}{dx}$
 $P^{2} = -\frac{h^{2}}{\Psi^{2}}(\frac{d\Psi}{dx})^{2}$
 $E = \frac{\rho^{2}}{2m} + V(x)$

Problem, con't



Can you explain why Schroedinger did not use this version instead??

Summary/Announcements

- We "derived" Schrodinger's equation!
- Next time:
 - Time-dependent Schrodinger Equation
 - Probabilities and boundary conditions
- There is a copy of textbook on reserve in the SERC Reading Room (downstairs)
- The first HW is due at the beginning of next Lecture (Wednesday).