Quantum Physics 1

Notes-6

The State Function

and its Interpretation

Important results so far

- Einstein− deBroglie relations: $p = \hbar k = \frac{h}{\lambda}; \quad E = \hbar\omega = hf$

  The probability interpretation: $P(x)dx = \Psi^*\Psi dx$

- $\langle q \rangle = \int \Psi^* q(x) \Psi dx$

  The general form for a wave packet using waves with

  well−defined momentum: $\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) e^{i(kx-\omega t)} dk$

  where $A(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0) e^{-ikx} dx$. This says that we can

  express any wavefunction as a sum of pure momentum states.

Introduction

- Observables are physical attributes of a system that can be measured in the laboratory.
- In quantum physics, in the absence of a measurement, a microscopic system does not necessarily have values of its physical properties. (A particle does not "have" a position until we measure it. It has a set of possible positions.)
- We want to find out how to calculate observables from wavefunctions. The mathematical approach is through the introduction of operators.

A Plausibility Argument for The Schrodinger Equation

- A starting point:
  1. The wave equation must be consistent with the two quantum postulates:
     - DeBroglie $\lambda = \frac{h}{p}$
     - And Einstein $E = hf (= \hbar\omega)$
  2. It must be consistent with
     - Kinetic energy + Potential Energy = Total energy: $\frac{p^2}{2m} + V = E$
  3. It must be linear so that the sum of two solutions is itself a solution.
     - If $\Psi_1 and\ \Psi_2 are\ solutions, then\ \Psi_{12} = \Psi_1 + \Psi_2\ is\ a\ solution$.

SE Plausibility

- Assume now that the potential is constant in time and space: $V(x,t) = V_0 = 0$
  - The classical expression for the force on a particle is $\vec{F} = -\vec{\nabla} V$ so the force on the particle would be zero.
  - If the force is zero, then the momentum and total energy are constants.
- $T + V = E$ (or $\frac{p^2}{2m} = E$) so using the Einstein and DeBroglie postulates
  - $\frac{h^2}{2m\lambda^2} = hf$ (or $\frac{\hbar^2 k^2}{2m} = \hbar\omega$)

SE Plausibility

- Since we want the wave equation to be linear, the wavefunction can only appear in the first order.
- Consider if a solution is a travelling wave:

$$\Psi = f(kx - \omega t) = f(u)$$

  - $\frac{\partial \Psi}{\partial x} = \frac{\partial \Psi}{\partial u}\frac{\partial u}{\partial x} = k\frac{\partial \Psi}{\partial u}$ and $\frac{\partial^2 \Psi}{\partial x^2} = k^2\frac{\partial^2 \Psi}{\partial u^2}$, so a second derivative in x produces the factor of k^2.
  - The first derivative in time produces a factor of ω.
  - Schrodinger therefore proposed that the wave equation had the form: $\alpha\frac{\partial^2 \Psi}{\partial x^2} = \beta\frac{\partial \Psi}{\partial t}$

The Schrodinger Equation

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

Two ways to compute momentum

1) Given $\Psi(x,t)$, use the wave function to compute $\Phi_p(p)$.

Compute $\langle p \rangle$ from $\int \Phi^* p \Phi dp$.

2) Find a way to express p as a function of x.

Compute $\langle p \rangle$ from $\int \Psi^* p(x) \Psi dx$.

Finding a Momentum Operator

- The Correspondence Principle states that the behavior of systems described by quantum mechanics must be consistent with classical physics in the appropriate limit.
- For example: $\frac{d\langle x\rangle}{dt} = \frac{\langle p_x\rangle}{m}$
- Let's follow through on this to see if we can find a simple operator that will yield $\langle p_x\rangle$ from the space representation of the wavefunction.

Finding a Momentum Operator

$$\frac{d\langle x\rangle}{dt} = \frac{d}{dt}\int_{-\infty}^{\infty} x\Psi^*\Psi dx = \int_{-\infty}^{\infty} x\frac{\partial\Psi^*\Psi}{\partial t}dx$$

And using the same Schrodinger eqn substitution as for the probability current,

$$\frac{d\langle x\rangle}{dt} = \int_{-\infty}^{\infty} x\frac{\partial}{\partial x}\left[\frac{i\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \Psi\frac{\partial\Psi^*}{\partial x}\right)\right]dx$$

Integrating by parts:

$$\frac{d\langle x\rangle}{dt} = \int_{-\infty}^{\infty}\left[\frac{i\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \Psi\frac{\partial\Psi^*}{\partial x}\right)\right]dx + \left[\frac{xi\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \Psi\frac{\partial\Psi^*}{\partial x}\right)\right]_{-\infty}^{\infty}$$

$$\frac{d\langle x\rangle}{dt} = \int_{-\infty}^{\infty}\left[\frac{i\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \Psi\frac{\partial\Psi^*}{\partial x}\right)\right]dx$$

Finding a Momentum Operator

$$\frac{d\langle x\rangle}{dt} = -\int_{-\infty}^{\infty}\left[\frac{i\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x}\right)\right]dx - \int_{-\infty}^{\infty}\left[\frac{i\hbar}{2m}\left(\Psi\frac{\partial\Psi^*}{\partial x}\right)\right]dx$$

Integrate second term by parts:

$$\frac{d\langle x\rangle}{dt} = -\frac{1}{m}\int_{-\infty}^{\infty}\left[\left(\Psi^*\frac{\hbar}{i}\frac{\partial\Psi}{\partial x}\right)\right]dx$$

And comparing with $\frac{d\langle x\rangle}{dt} = \frac{\langle p_x\rangle}{m}$, we find that:

$\langle p_x\rangle = \int_{-\infty}^{\infty}\left[\left(\Psi^*\frac{\hbar}{i}\frac{\partial\Psi}{\partial x}\right)\right]dx$ so an operator that produces the momentum expectation value is

$$\boldsymbol{p_{op} = \frac{\hbar}{i}\frac{\partial}{\partial x}}$$

Checking the Momentum Operator

Consider a pure momentum state:

$$\Psi(x,t) = Ae^{i(px-Et)/\hbar}$$

And using the momentum operator:

$$\mathrm{p_{op}}\Psi = \frac{\hbar}{i}\frac{\partial\Psi}{\partial x} = \frac{\hbar}{i}A\frac{ip}{\hbar}e^{i(px-Et)/\hbar} = p\Psi$$

Some other operators

To find the expectation value of a general observable: Q.

First construct an operator to extract Q, $\hat{Q}$.

(For wavefunctions, this can usually be accomplished by rewriting the physical quantity in terms of x and p.)

Then compute the expectation integral as before

$$\langle Q \rangle = \int \Psi^* \hat{Q}(x) \Psi dx$$

Some other operators

Classical kinetic energy $T = \frac{p^2}{2m}$

(When an operator is squared, that means to perform the operation twice)

$$\hat{T}\psi = \frac{1}{2m}\hat{p}^2\psi = \frac{1}{2m}\hat{p}\hat{p}\psi = \frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x}\right)\left(-i\hbar\frac{\partial}{\partial x}\right)$$

$$= \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi$$

Position: $\hat{x} = x$

Constant: $\hat{C} = C$

Solving the Schrodinger Equation

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

If the potential energy is independent of time, then we can start solving this equation using the separation of variables technique:

- Assume that $\Psi(x,t)=\psi(x)f(t)$

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

$$-\frac{1}{\psi(x)}\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}+V(x)\psi(x)=i\hbar\frac{1}{f(t)}\frac{\partial \mathrm{f(t)}}{\partial t}$$

And the only way the two sides can be equal for a x and t is if they are equal to a constant (which we will call *E*)

Solving the Schrodinger Equation

$$-\frac{1}{\psi(x)}\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}+V(x)\psi(x)=i\hbar\frac{1}{f(t)}\frac{\partial f(t)}{\partial t}=E$$

Solving $i\hbar\frac{1}{f(t)}\frac{\partial f(t)}{\partial t}=E$, $\frac{df(t)}{f(t)}=-i\frac{E}{\hbar}dt$ and integrating both sides:

$$\ln\big(f(t)\big)-\ln\big(f(0)\big)=-i\frac{E}{\hbar}t$$

$$f(t)=Ce^{-i\frac{E}{\hbar}t}=Ce^{-i\omega t}$$

And the left hand side:

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

Is known as the time-independent Schrodinger Equation

Solution for $\psi(x)$ for constant V(x)

$$\frac{\partial^2\psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V)\psi(x) = 0$$

And setting $k^2 = \frac{2m}{\hbar^2}(E - V)$ for $E > V$

$$\frac{\partial^2\psi(x)}{\partial x^2} + k^2\psi(x) = 0$$

Which has solutions:

$\psi(x) = Ae^{ikx}$and Be^{-ikx}

So the overall solution is:

$\Psi(x,t) = Ae^{-i(kx+\omega t)} + B\ e^{i(kx-\omega t)}$

Traveling waves!

Particle in a well with infinite walls

- $V(x) = 0 \; for \; 0 < x < L$ and infinity for $|x| > L$.
- Inside the well:
  $\Psi(x,t) = (Ae^{-i(kx)} + B\, e^{i(kx)})\, e^{-i\omega t}$
- Boundary conditions:

$\psi(x) = 0 \; at \; x = 0 \; and \; x = L$

$\psi(0) = 0 \;\rightarrow\; A + B = 0$ so $-A = B$

$\psi(x) = A(e^{-i(kx)} - e^{i(kx)}) = -Asin(kx)$

$\psi(L) = 0 \;\rightarrow\; Asin(ka) = 0 \;\rightarrow\; ka = n\pi$

$k_n = n\frac{\pi}{a}$ where n is an integer. (quantization)

Particle in a well

$k^2 = \frac{2m}{\hbar^2}E \quad and \quad k^2 = \frac{n^2\pi^2}{L^2}$ so

$E_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2} = \frac{h^2 n^2}{8mL^2}$ (quantized)

Another way of finding this result:

λ that meets the boundary conditions must be such that $\frac{n\lambda_n}{2} = L$ and since $p = \frac{h}{\lambda}$ and $E = \frac{p^2}{2m}$ we have $E = \frac{h^2 n^2}{8mL^2}$.

The formal TISE approach allows us to deduce a lot more physics.