

Quantum Physics 1

Notes-6 The State Function and its Interpretation

Important results so far

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

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.

Important results so far

- Probability Current Density

$$-\frac{i\hbar}{2m} \left(\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x} \right) \equiv j_x(x)$$

- For a pure momentum wave of amplitude, A, the

probability current density is $\frac{|A|^2 p_0}{m} = \hbar \frac{|A|^2 k_0}{m}$

- Heisenberg Uncertainty: $\Delta x \Delta p \geq \frac{\hbar}{2}$.
- Time evolution of the wavepacket:

Given: $A(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x, 0) e^{-ikx} dx,$

then $\Psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) e^{-i(kx - \omega(k)t)} dk.$

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 Ψ_1 and Ψ_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

It is then a question of finding coefficients that are consistent with the Einstein-DeBroglie Relations

The result:

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

Two ways to compute momentum

1) Given $\Psi(x, t)$, use the wave function to compute $\Phi_p(p)$. (*e.g. – by Fourier Transform*)

Then 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:

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

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

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

Checking the Momentum Operator

Consider a pure momentum state:

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

And using the momentum operator:

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

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)

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

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 $\Psi(x, t) = \psi(x)f(t)$

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

And the only way the two sides can be equal for all 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:

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

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

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:

$$\psi(x) = Ae^{ikx} \text{ and } Be^{-ikx} \text{ (or } A' \sin kx + B' \cos kx)$$

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:

$$\psi(x) = 0 \text{ at } x = 0 \text{ and } x = L$$

$$\psi(0) = 0 \rightarrow A + B = 0 \text{ so } -A = B$$

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

$$\psi(L) = 0 \rightarrow A\sin(ka) = 0 \rightarrow ka = n\pi$$

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

Particle in a well

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

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

[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.]