Quantum Physics 1

Class 3

The State Function and its Interpretation

Townsend Ch 2.3-2.4

In a particle-detection scheme, the wave-like interference pattern builds up particle-by-particle

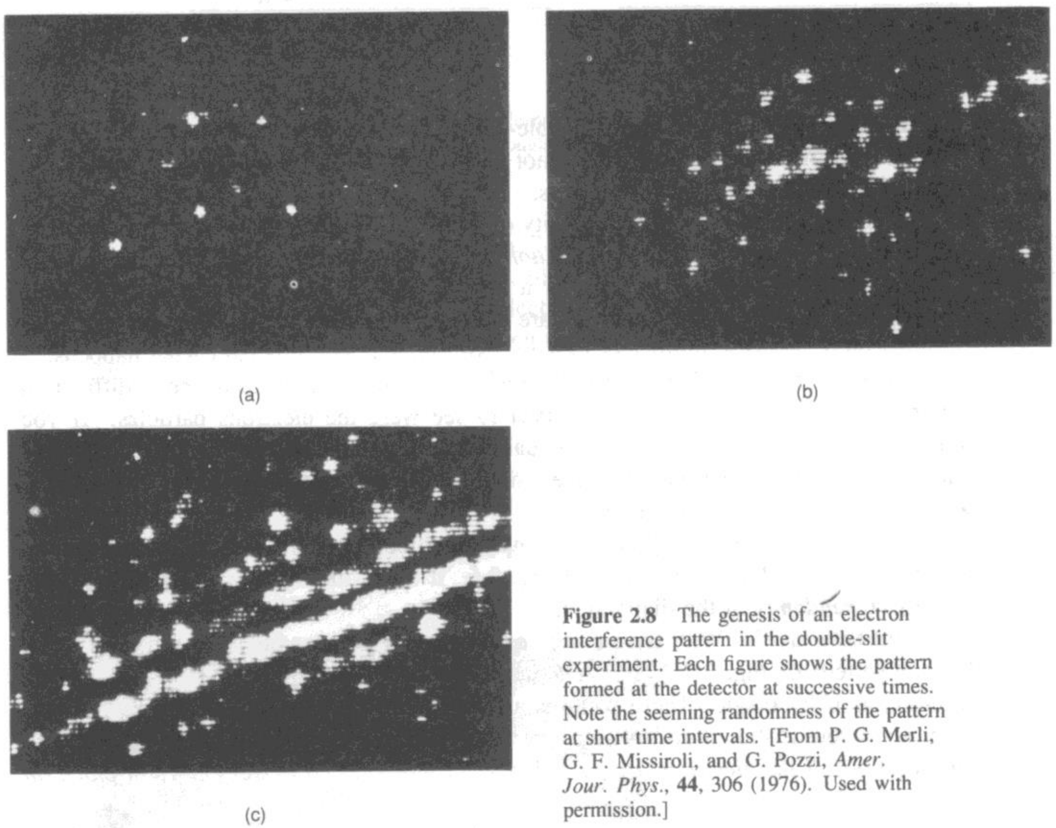


Figure 2.8 The genesis of an electron interference pattern in the double-slit experiment. Each figure shows the pattern formed at the detector at successive times. Note the seeming randomness of the pattern at short time intervals. [From P. G. Merli, G. F. Missiroli, and G. Pozzi, *Amer. Jour. Phys.*, **44**, 306 (1976). Used with permission.]

from Morrison

- Note that the arrival of each particle appears to be random, until enough particles have arrived for a statistically useful sample.
- This suggests that we should use a **probability distribution** approach for quantum physics calculations

Discussion of probability

- The word **event** refers to obtaining a measurement of an observable.
- To define the **probability** of an event result, we consider the fraction of times that result will occur for measurements on a very large number of identical systems. Such a collection of systems is called an **ensemble**.
- To perform an **ensemble measurement** of an observable, we perform precisely the same measurement on the members of an ensemble of identical systems.

Normalized Probability

The probability of a specific outcome is the number of times that it occurs, divided by the total number of experiments:

$$P(a) = \frac{n_a}{N}$$

The probability of a set of outcomes is the sum of the probabilities of each outcome:

$$P(a \text{ or } b \text{ or } \ldots) = \sum_{j=a}^{c} P(j) = \frac{1}{N} \sum_{j=a}^{c} n_j$$

By this definition, all possible outcomes must have a total probability of one

$$\sum_{j=a} P(j) = 1$$

Ensemble Averages

- Given the probabilities for a set of outcomes, we can find useful quantities, like the average*
(or expectation value) of a result *q*, through a simple sum:

$$\text{"mean of q"} = \langle q \rangle = \bar{q} = \frac{\sum_{j=1}^{M} q_j P(q_j)}{\sum_{j=1}^{M} P(q_j)}$$

- Another statistic that is useful in describing distributions is the dispersion or variance:

$$\text{variance} = \text{dispersion} = \langle (q - \langle q \rangle)^2 \rangle$$

*Physics words: average=mean=expectation value

Continuous distributions

- In many physical cases, the result of a measurement can be <u>any</u> value within a physical range, for example, the position of a particle.
- We can define the probability of finding the particle within a certain infinitesimal range as *P(x)dx* and we call *P(x)* the **<u>probability density</u>.**
- Given a probability density, we can compute the **<u>expectation value</u>** of any parameter *q(x)*.

$$\langle x \rangle = \int_{-\infty}^{\infty} x P(x) dx$$

$$\langle q(x) \rangle = \int_{-\infty}^{\infty} q(x) P(x) dx$$

Matter waves

- Just adding probability distributions does not give interference.
- In order to get an interference pattern, we must be able to superpose two waves.
- A working hypothesis:
  - Observations occur in proportion to the probability that a particle will be in a state (r(t), p(t), E(t)) when it is measured.
  - The probability is proportional to the square of a wave amplitude.

The State Function

- Every physically realizable state of a system is described in quantum mechanics by a **state function** Ψ that contains all *accessible* information about the system in that state.

  – The phrase “**wave function**” is usually used to mean a state function that is specified as a function of position and time $\Psi(x,t)$.

Born's Postulate

If, at time t, a measurement is made to locate the particle associated with the wavefunction $\Psi(\vec{r},t)$, then the probability $P(\vec{r},t)dv$ that the particle will be found in the volume dv around position $\vec{r}$ is equal to

$$\boldsymbol{P(\vec{r},t)dv = \Psi^*(\vec{r},t)\Psi(\vec{r},t)dv}.$$

Where $\Psi^*(\vec{r},t)$ denotes the complex conjugate of $\Psi(\vec{r},t)$.

Principle of Superposition

If Ψ_1 and Ψ_2 represent two physically realizable states of
a system, then the linear combination
$\Psi = c_1\Psi_1 + c_2\Psi_2$
is also a physically realizable state of the system.

Normalization

- Sometimes you will be given wave functions that lead to an integrated probability that is not already 1. (or that have an unspecified multiplicative constant.)
- Before you try to do any calculation with a wavefunction, you should decide whether it needs to be <u>normalized</u> so that the integrated probability is 1.

Given an un−normalized wavefunction Ψ' such that $\int_{-\infty}^{\infty} \Psi' * (\vec{r},t)\Psi'(\vec{r},t)dv = M$

just multiply Ψ' by the constant $\frac{1}{\sqrt{\mathrm{M}}}$ to create a new function:

$\Psi(\mathrm{x,t}) = \frac{\Psi'(\mathrm{x,t})}{\sqrt{M}}$ that will be normalized.

A quick peek at the Schrodinger Equation

Later, we will deduce and solve the wave equation for matter waves (The Schrodinger Equation).
Here I will show it to you, make some simplifying assumptions, and discuss the nature of the solutions.
Here it is, in one dimension,

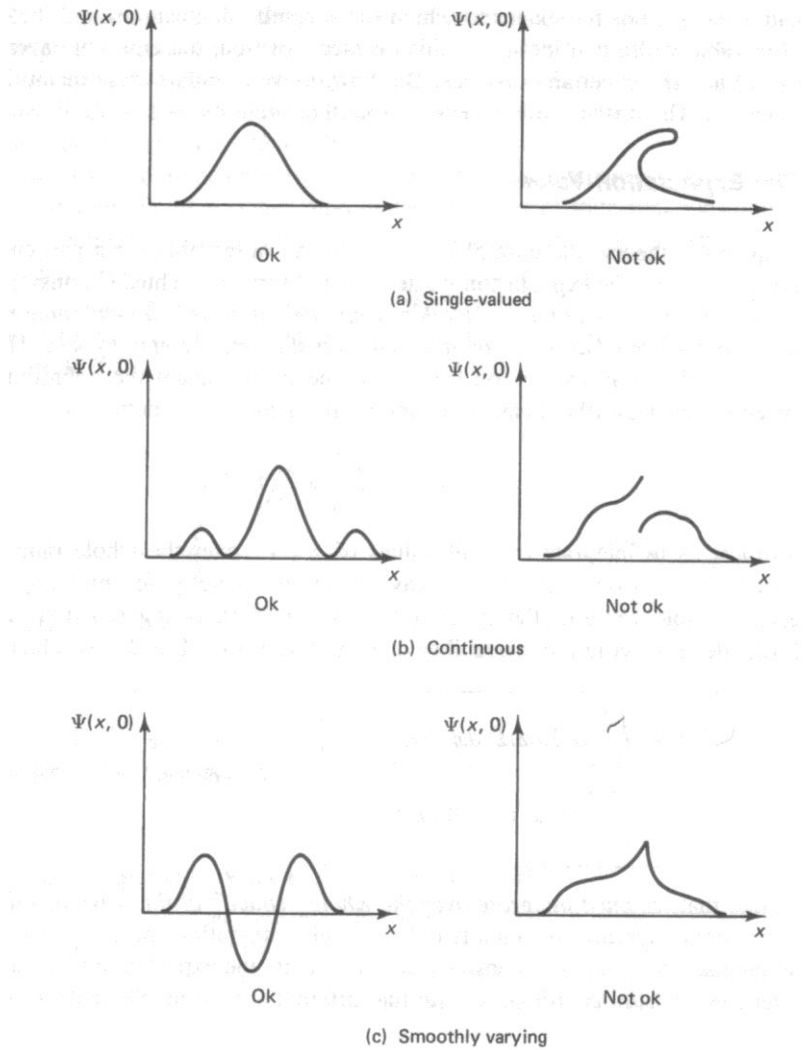
$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right]\Psi(x,t)=i\hbar\frac{\partial\Psi(x,t)}{\partial t}$$

and in 3: $\left[-\frac{\hbar^2}{2m}\vec{\nabla}^2+V(\vec{r})\right]\Psi(\vec{r},t)=i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t}$

Physical constraints on wavefunctions

- A physical wavefunction must be normalizable. (The particle must be somewhere.)
- A physical wavefunction must be single valued. (It can’t have two probabilities of being at the same point.)
- A physical wavefunction and its spatial derivatives must be continuous.

Examples of allowed and disallowed wavefunctions



(from Morrison)

Expectation value

- In quantum mechanics, the ensemble average of an observable for a particular state of the system is called the **expectation value** of that observable.

$$\langle Q \rangle = \frac{\int_{-\infty}^{\infty} \Psi^* Q \Psi dv}{\int_{-\infty}^{\infty} \Psi^* \Psi dv}$$

- The **uncertainty** in the observable is the square root of the variance

$$\Delta Q = [\langle (Q - \langle Q \rangle)^2 \rangle]^{1/2} = [\langle Q^2 \rangle - \langle Q \rangle^2]^{1/2}$$

Einstein-de Broglie relations

As we continue to analyze behavior of wavefunctions it is useful for us to keep in mind two basic relations for matter waves, relating particle properites to wave properties:

$$E = hf = \hbar\omega$$

and

$$p = \frac{h}{\lambda} = \hbar k$$

Free space solution for Ψ

For V(x)=0, we can illustrate some physical points by working through the wave function logic of this physical situation without fully solving the differential equation.

A. If Ψ is to be normalizable, it must go to zero as $r \to$ infinity.

B. Ψ must be complex, because the right side of the SE has an inescapable *i* in it.

C. Ψ must not violate the homogeneity of free space. (The probability must be the same after we translate Ψ by an arbitrary distance.)

Three trial functions

1) $\Psi(x,t) = A\cos(kx - \omega t + \varepsilon)$:a real harmonic wave
2) $\Psi(x,t) = Ae^{i(kx-\omega t)}$:a complex harmonic wave
3.) A complex wavepacket

A. Ψ normalizable?

B. Ψ complex?

C. Ψ must not violate the homogeneity of free space.

Test the harmonic function

$\Psi(x,t) = A\cos(kx - \omega t + \varepsilon)$:a real harmonic wave

A. Normalizable? No, unless A goes to zero.

B.) Complex? No. Unlikely to satisfy the wave equation.

C.) Homogeneous P? No.

$$P(x,t) = \Psi^*(x,t)\ \ \Psi(x,t) = A^2\cos^2(kx - \omega t + \varepsilon)$$

$$P(x+a,t) = \Psi^*(x+a,t)\ \ \Psi(x+a,t)$$

$$\Psi(x+a,t) = A[\cos(kx - \omega t)\cos k\,a + \sin(kx - \omega t)\sin k\,a]$$

$$P(x+a,t) = P(x,t)\cos^2 k\,a +$$
$$+A^2[\sin^2(kx - \omega t)\sin^2 k\,a + 2\cos k\,a\sin k\,a\cos(kx - \omega t)\sin(kx - \omega t)]$$
$$\neq P(x,t)$$

Test the complex harmonic function

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

A. Normalizable? Only if A goes to zero.

$$\int \mathrm{P(x,t)dx} = \int Ae^{-i(kx-\omega t)}Ae^{i(kx-\omega t)}dx = \int_{-\infty}^{\infty} A dx$$

$= A[2\infty]$

B.) Complex? Yes. It is indeed a solution to

C.) Homogeneous P? Yes.

$P(x,t) = \Psi(x,t)^*\Psi(x,t)$

$= A^2$ (independent of position)

We seem to be on the right track.

The complex wave packet

We can construct a localized/normalizable wavepacket out of complex harmonic waves using the Fourier transform:

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

⇒ Because this wavefunction can be localized, it is likely to be normalizable. (We will need to test specific cases.)

⇒ Because each term in it is a solution to the wave equation, the wave function must also be a solution.

⇒ Is the shape of the probability of the sum of complex harmonics translation invariant?

$$P(x,t) = \left(\tilde{a}e^{ik_1x} + \tilde{b}e^{ik_2x}\right)^*\left(\tilde{a}e^{ik_1x} + \tilde{b}e^{ik_2x}\right)$$

$$= \left(\tilde{a}^*e^{-ik_1x} + \tilde{b}^*e^{-ik_2x}\right)\left(\tilde{a}e^{ik_1x} + \tilde{b}e^{ik_2x}\right)$$

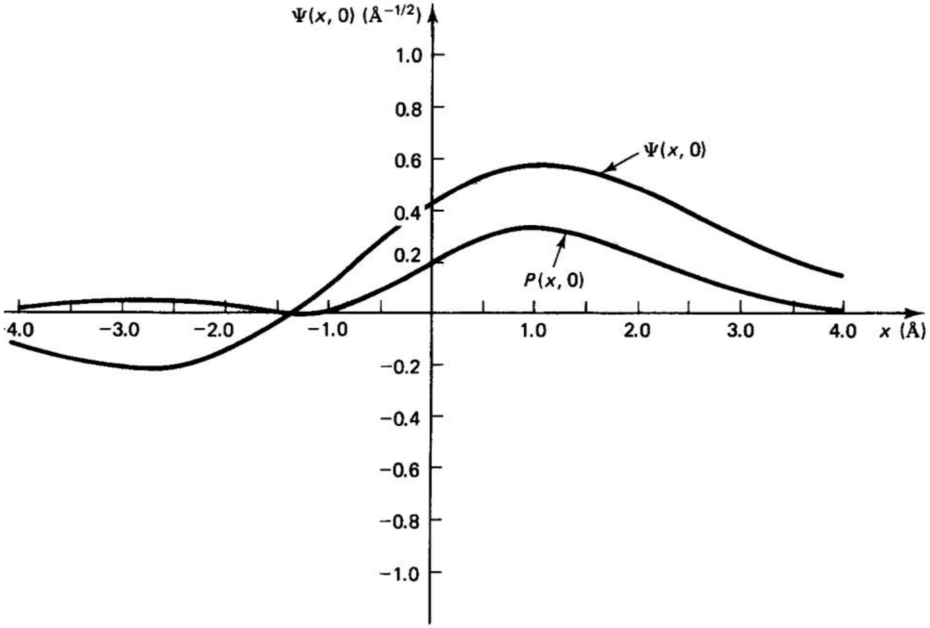
$$= a^2 + b^2 + \tilde{a}^*\tilde{b}e^{-i(k_1-k_2)x} + \tilde{b}^*\tilde{a}e^{i(k_1-k_2)x} = a^2 + b^2 + \tilde{a}^*\tilde{b}e^{-ik\prime x} + \tilde{b}^*\tilde{a}e^{ik\prime x}$$

$$P(x+\alpha,t) = a^2 + b^2 + \tilde{a}^*e^{-ik_1x-ik_1\alpha}\tilde{b}e^{ik_2x+ik_2\alpha} + \tilde{b}^*e^{-ik_2x-ik_2\alpha}\tilde{a}e^{ik_1x+ik_1\alpha}$$

$$= a^2 + b^2 + \tilde{a}^*\tilde{b}e^{-ik\prime(x+\alpha)} + \tilde{b}^*\tilde{a}e^{ik\prime(x+\alpha)}$$

<u>This function is just the old one, moved over.</u>

In-class exercise 1



- Morrison 3.1 p. 89

This is a normalized state function at t=0.

The magnitude of Ψ(x,0) continues to decay smoothly to zero as $x \to \pm\infty$.

1. Is this function physically admissible? Why or why not?
2. Where is the particle most likely to be found?
3. Estimate the expectation value of the position. Is it the same as for part 2?
4. Is the uncertainty in momentum of this state equal to zero? Justify.

In-class discussion and questions 2

- Morrison 3.3 p. 90

3.3 Measurement in Quantum Mechanics: Short-Answer Questions

Consider a system whose state function $\Psi(x,t)$ at a fixed time t_0 is shown in Fig. 3.3.1.

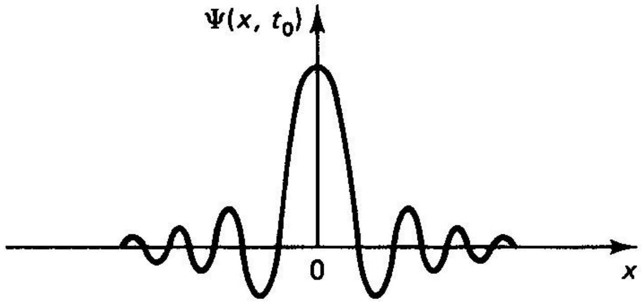


Figure 3.3.1

(a) **Describe** how you would calculate the expectation value of position for this state from the functional form of $\Psi(x,t)$.

(b) What is the value of ensemble average of position for this state at time t_0?

(c) **Describe** briefly how you would calculate the position uncertainty for this state from $\Psi(x,t)$.

(d) Is Δx zero, positive-but-finite, or infinite? Why?

(e) Is the momentum uncertainty Δp zero, positive but finite, or infinite? Why?

(f) Can this state function be normalized? If not, why not? If so, describe briefly how you would normalize $\Psi(x,t)$.

Summary:
(In which I try to clarify what we are doing)

- From evidence of interference in “particle” experiments, we introduced the idea that matter must be described by some sort of wave.
  - De Broglie-Einstein relations: $p=h/\lambda$; $E=hf$
- The wave is <u>not directly observable</u>, but the resulting probability of various outcomes is, hence we introduced a probability interpretation of quantum physics experiments.
- We then assumed that there existed a wave that could yield the correct observables, with classical relations between time, energy, momentum, and position. The ramifications were then explored.
  - The probability of an outcome is proportional to the square of the wavefunction for that outcome.
  - The probability interpretation leads to the ability to compute the expectation (average) value and variance for appropriate observables once the wave function is known.
  - The superposition of waves to form a packet leads to a mathematical statement of the Heisenberg Uncertainty Principle.
  - We could deduce the form of a useful wave equation for matter waves.
- We will next explore some examples of wave functions and their observable ramifications.
  - Wavepackets, momentum-position transforms
  - More general state functions – the momentum state