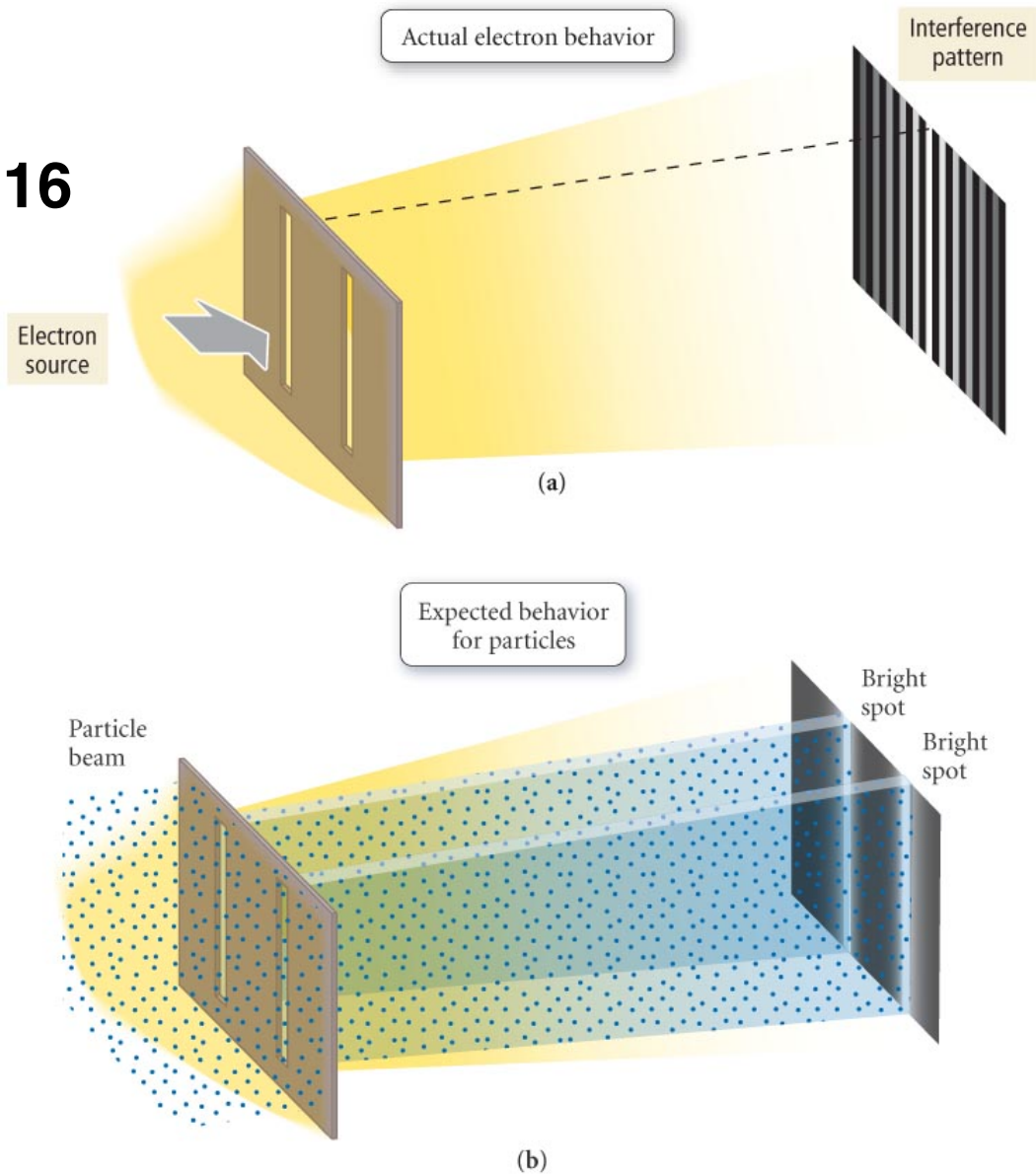
7.4 The Wave Nature of Matter

- Summary of Quantum Theory so far:
  - Energy levels of atoms are quantized
  - The energy of light is proportional to its frequency
  - As well as being a wave, light also has particle nature (photons).
- But does an object also have wave nature?
- De Broglie proposed that electrons do have properties of waves.
- This explained why electrons are restricted to certain orbits.

Electron Diffraction

Figure 7.16



de Broglie Wavelength

- $E = \frac{hc}{\lambda} = mc^2$ so: $\lambda = \frac{hc}{mc^2}$ or $\frac{h}{mc}$
- The **de Broglie wavelength** for an object is inversely proportional to its momentum:

$$\boldsymbol{\lambda = \frac{h}{m \cdot u}}$$

(Note: 1 J = 1 kg m^2/s^2, so h has units of kg m^2/s)

7.5 Quantum Mechanics

Heisenberg Uncertainty Principle:

- Due to its wave nature, It is impossible to know a particle's exact position *and* momentum.
- We cannot know for sure where an electron is located, only its *probability* of being in a certain position.
- A new theory was developed to take these ideas into account, called **quantum mechanics**.
- **Schrödinger Equation**:

$$\mathbf{H\Psi = E\Psi}$$

- The **wavefunctions** (Ψ) describe the motion of the electron, and its corresponding energy.
- The solutions of the Schrödinger equation give the different energy states for an atom, and the corresponding wave functions for each.

Quantum Mechanics (contd.)

- The value of Ψ^2 at a certain location gives the probability of finding the electron there.
- This leads to the formulation of **atomic orbitals**, the regions in space where the electron is "likely" to be located.
- Atomic orbitals are described by **quantum numbers**:

1. Principal quantum number, n

- n is a positive integer (1, 2, 3…)
- n determines the overall size and energy of orbital.
- Different n levels are referred to as **shells**.

2. Each shell can have a certain number of **subshells**, orbitals with different shapes.

Quantum Mechanics (contd.)

- Subshells are represented by letters:

- Only certain atomic orbitals exist. In any shell with a quantum number n, there are n subshells.
- Allowed atomic orbitals:

Quantum Mechanics (contd.)

3. In some subshells, there are atomic orbitals pointing in different directions. The third quantum number defines the direction. The number of atomic orbitals with different directions depends on the type of subshell:

- *s* subshells contain 1 atomic orbital.
- *p* subshells contain 3 atomic orbitals.
- *d* subshells contain 5 atomic orbitals.
- *f* subshells contain 7 atomic orbitals.

4. There is a fourth quantum number called the **magnetic spin quantum number** (m_s). An electron can have two possible values of spin, often called "up" or "down."

- The spin quantum number does not determine the atomic orbital; it only describes a property of an electron.

7.6 The Shapes of Atomic Orbitals

- *s* orbitals are **spherical**.

Figure 7.23

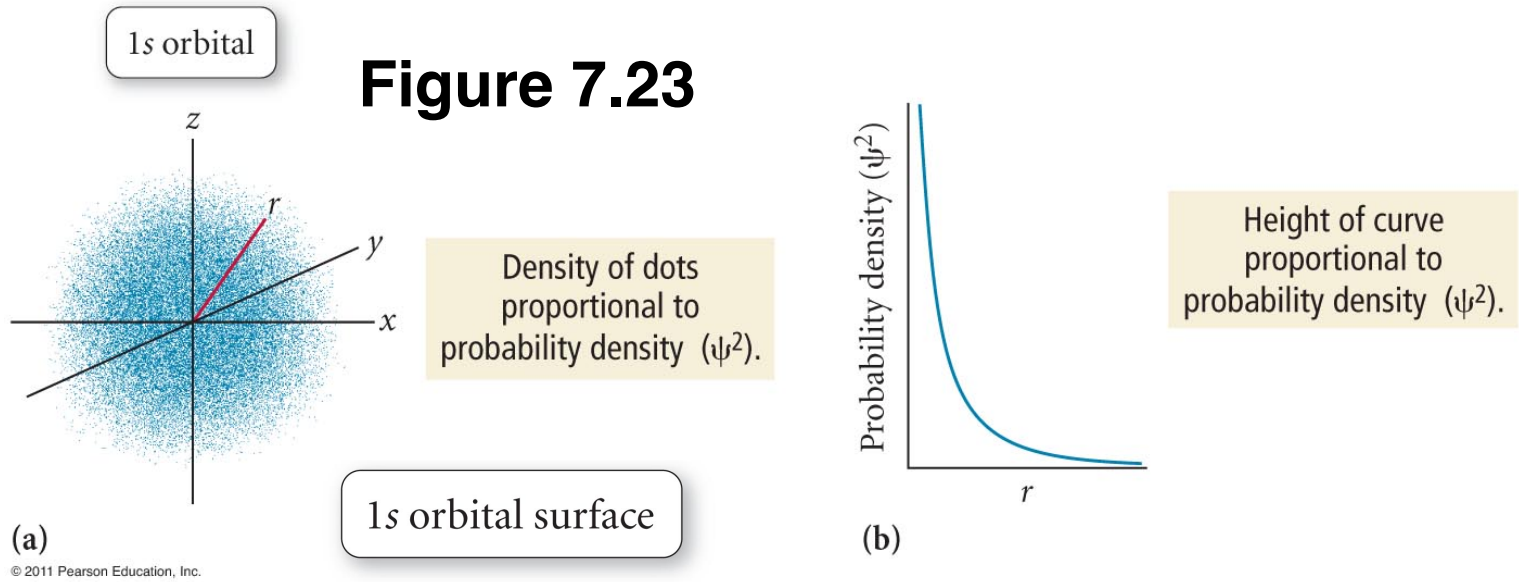
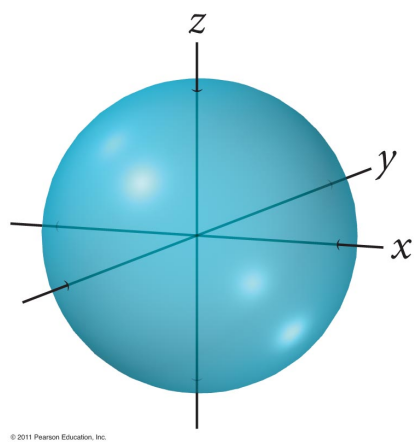


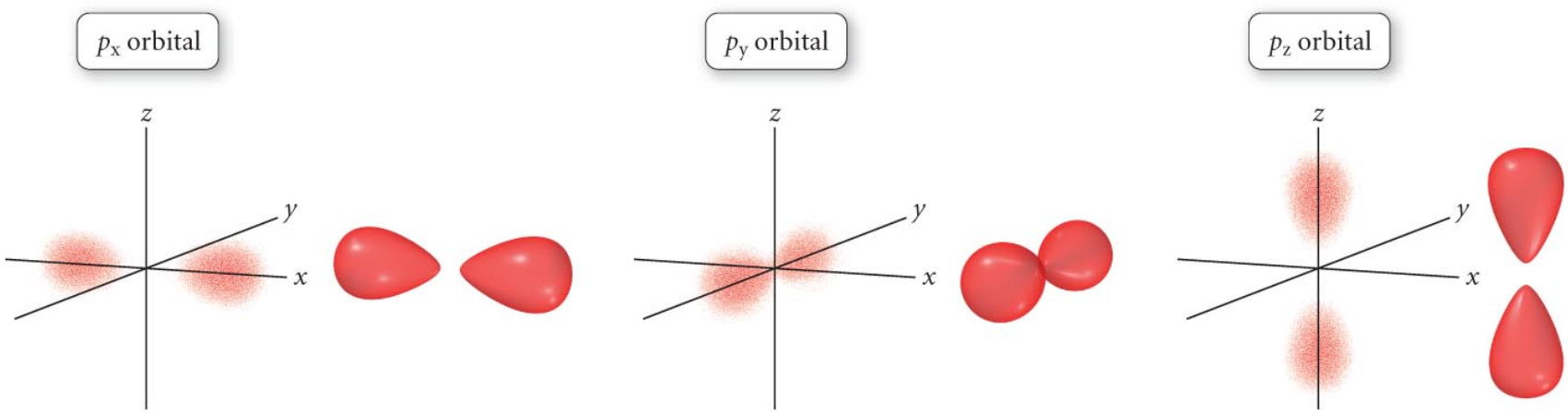
Figure 7.24



The Shapes of Atomic Orbitals (contd.)

- *p* orbitals consist of two lobes, separated by a **node**.
  - A wavefunction has a value of zero at a node, so an electron will <u>never</u> be found there.
- There are three *p* orbitals, each pointing in a different direction: p_x, p_y, p_z

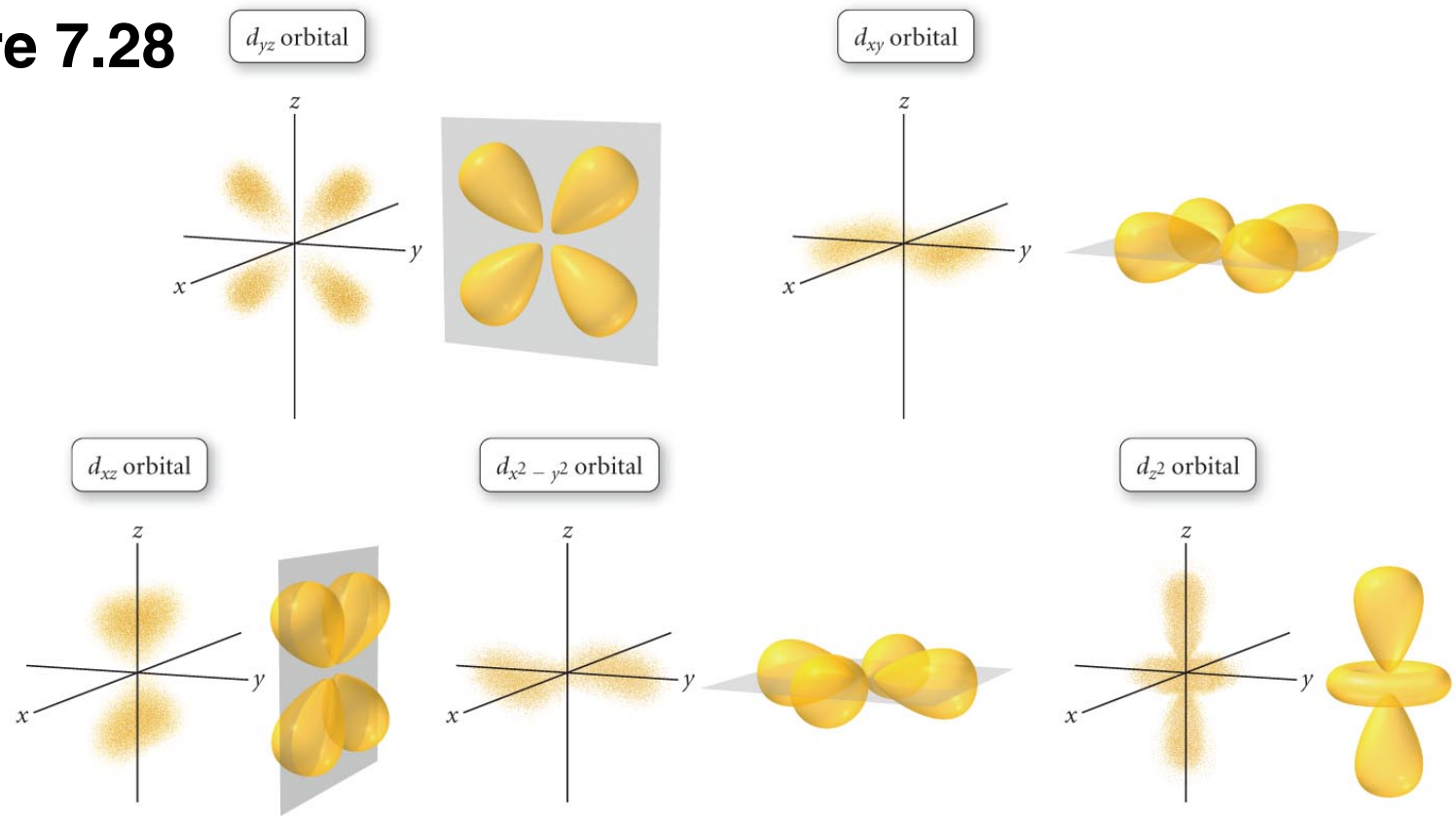
Figure 7.27



The Shapes of Atomic Orbitals (contd.)

- The five 3*d* orbitals:
- In general: four lobes, two nodes.

Figure 7.28



The Shapes of Atomic Orbitals (contd.)

- There are seven 4*f* orbitals:

Figure 7.29