Schaum's Outline Series
Modern Physics.

Chapter 23

The Pauli Exclusion Principle

23.1 INTRODUCTION

To this point we have considered quantum mechanical systems possessing many energy levels but only one effective electron, namely hydrogenlike atoms. We have found that in the absence of strong spin-orbit coupling the behavior of the electron is described by specifying the values of its four quantum numbers (n, l, m_l, m_s) that are respectively associated with its energy, orbital angular momentum, the z-component of the orbital angular momentum, and the z-component of its spin. When these four quantum numbers are given it is said that the *state* of the (one-electron) system has been specified.

In this and the following chapters we shall describe quantum mechanical systems that have many energy levels and *more than one electron*.

23.2 THE PAULI EXCLUSION PRINCIPLE

By analyzing spectroscopic data from atoms with more than one electron, Wolfgang Pauli in 1924 came to the conclusion that in a quantum mechanical system *no two electrons can occupy the same state*. This result is called the *Pauli exclusion principle*; put another way, it states that no two electrons can have the same set of quantum numbers (n, l, m_l, m_s).

The Pauli exclusion principle correlates many important experimental facts of atomic structure and provides the explanation of the periodic table of the elements, the subject of Chapter 24. To illustrate the Pauli exclusion principle, however, we will here discuss the simple problem of one or more particles of mass m moving in a straight line and confined between the points 0 and a, i.e. particles in a one-dimensional "box" of length a.

23.3 A SINGLE PARTICLE IN A ONE-DIMENSIONAL BOX

The problem of a single particle in a one-dimensional box was solved previously in Problem 17.3. It was found that the energy of the particle could not vary continuously, but could have only the discrete values given by

$$E_n = n^2 \frac{h^2}{8ma^2} \qquad n = 1, 2, 3, \ldots$$

Figure 23-1(a) shows these energy levels. We now take the particle in the box to be an electron with intrinsic spin. The state of the system is then specified by the pair of quantum numbers (n, m_s). In Fig. 23-1(b) the electron is in the $n=1$ state with "spin up" ($m_s = +\frac{1}{2}$); in Fig. 23-1(c) it is in the $n=3$ state with "spin down" ($m_s = -\frac{1}{2}$).

23.4 MANY PARTICLES IN A ONE-DIMENSIONAL BOX

The Pauli exclusion principle will have an important effect on the situation when more than one particle is in the one-dimensional box. In the following we assume that the energy levels are not altered when more than one particle is present.

With two electrons, the ground (lowest-energy) state of the system will have both electrons in the $n = 1$ energy level, one with spin up $(1, +\frac{1}{2})$ and one with spin down $(1, -\frac{1}{2})$, as shown in Fig. 23-2(a). Note that the two electrons do *not* have the same set of quantum numbers (n, m_s).

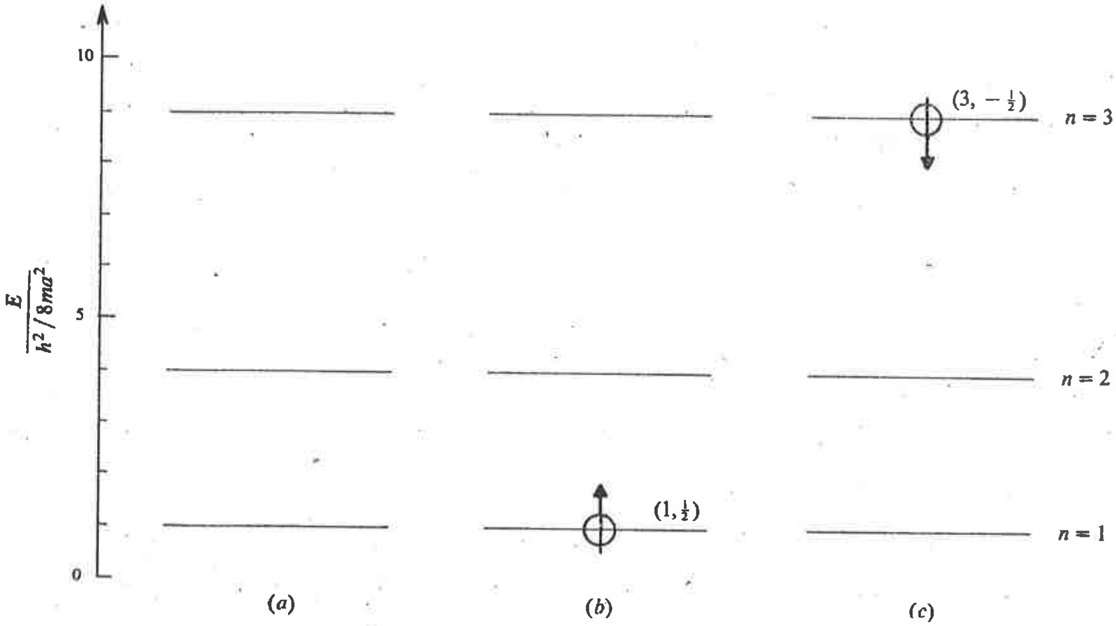


Fig. 23-1

Now consider what happens when a third electron is added to the system. The Pauli exclusion principle prohibits this electron from occupying the $n = 1$ energy level; for if it were in the $n = 1$ level, two of the three electrons would have the same set of quantum numbers (n, m_s). The third electron must therefore go to a *different* energy level, the $n = 2$ level if the system is in its ground state, as shown in Fig. 23-2(*b*) for a spin up configuration.

A similar line of reasoning shows that a fourth electron can be put into the $n = 2$ level, but when a fifth is added it must go into the $n = 3$ level, as shown in Fig. 23-2(*c*) for a spin down configuration. Thus it is seen that the Pauli exclusion principle has the effect of increasing the total energy of the

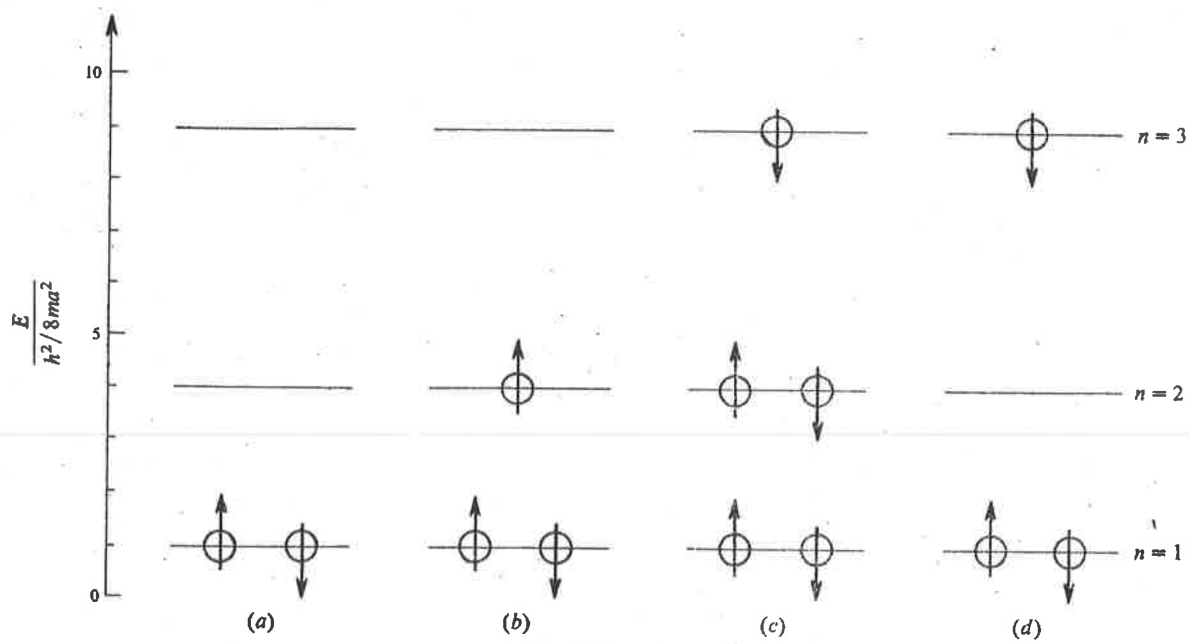


Fig. 23-2

ground state of the system to a much higher value than it would have if all the electrons occupied the $n = 1$ energy level.

Excited states of the above systems occur when the electrons do not occupy all the lowest available energy levels, as shown for a three-electron system in Fig. 23-2(*d*). As with one-electron systems, it is possible for energy in the form of photons to be emitted when excited electrons seek their ground state configurations.

Solved Problems

23.1. Calculate the first three energy levels for noninteracting electrons in an infinite square well of length 6 Å.

The energy levels are given by

$$E_n = \frac{n^2h^2}{8ma^2} = \frac{n^2(hc)^2}{8(mc^2)a^2} = \frac{n^2(12.4 \times 10^3\ \text{eV}\cdot\text{Å})^2}{8(0.511 \times 10^6\ \text{eV})(6\ \text{Å})^2} = 1.04n^2\ \text{eV}$$

Therefore, $E_1 = 1.04$ eV, $E_2 = 4.16$ eV, $E_3 = 9.36$ eV.

23.2. What are the energies of the photons that would be emitted when the four-electron system in Fig. 23-3(*a*) returns to its ground state?

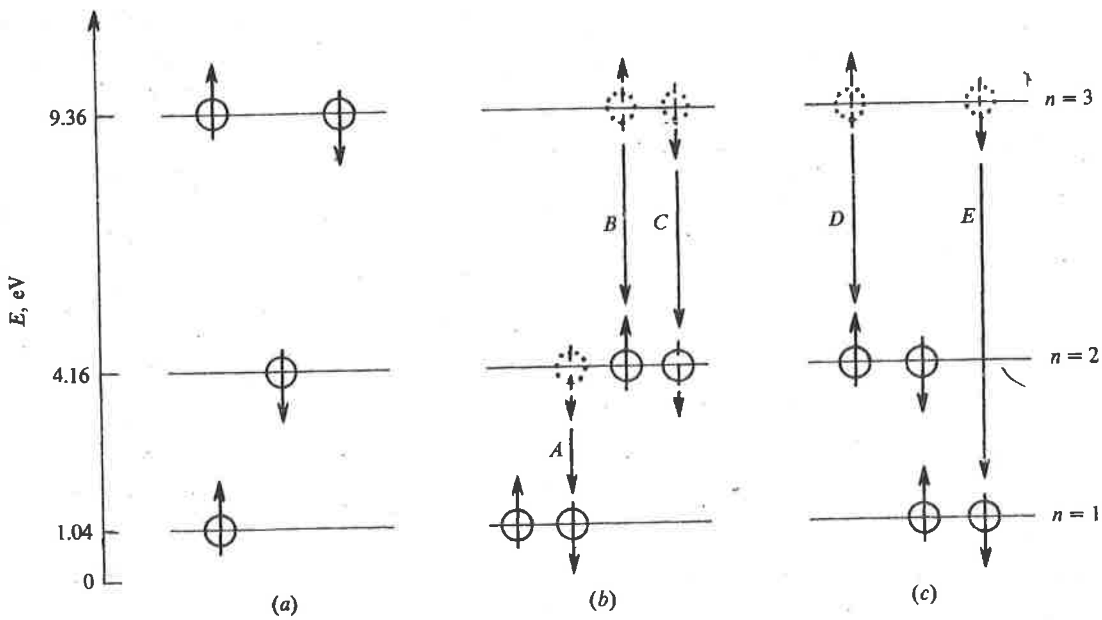
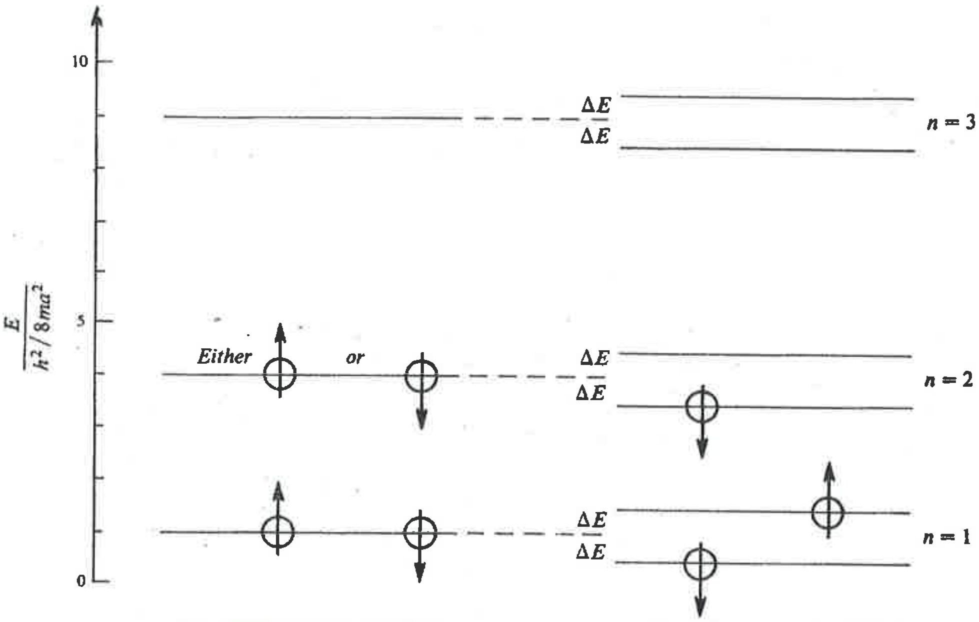


Fig. 23-3

The possible transitions that will return the system to its ground state are shown in Fig. 23-3(*b*) and (*c*). The energy of the emitted photon will be equal to the energy difference between the initial and final levels. Transitions *B*, *C*, and *D* have the same energy difference and therefore give rise to the same-energy photon.

$$E_A = E_2 - E_1 = 4.16\ \text{eV} - 1.04\ \text{eV} = 3.12\ \text{eV}$$
$$E_B = E_C = E_D = E_3 - E_2 = 9.36\ \text{eV} - 4.16\ \text{eV} = 5.20\ \text{eV}$$
$$E_E = E_3 - E_1 = 9.36\ \text{eV} - 1.04\ \text{eV} = 8.32\ \text{eV}$$

23.3. Consider three noninteracting particles in their ground states in an infinite square well [Fig. 23-4(a)]. What happens when a magnetic field is turned on which interacts with the spins of the particles?



(a) Without magnetic field (b) With magnetic field

Fig. 23-4

After the external magnetic field is applied, the new value (E_i) of each particle's energy equals the original value (E_n) plus the interaction energy:

$$E_i = E_n - \boldsymbol{\mu}_s \cdot \mathbf{B} = E_n - \mu_{sz} B = E_n + m_s \frac{e\hbar}{m} B$$

(see Problem 22.3). Since $m_s = \pm\frac{1}{2}$, the new levels will be displaced from the old by an amount $\Delta E = \pm e\hbar B/2m$, with a spin $-\frac{1}{2}$ particle occupying the lower sublevel and a spin $+\frac{1}{2}$ particle occupying the upper sublevel [Fig. 23-4(b)]. In contrast to the situation without the magnetic field present, the particle in the $n = 2$ level will have its spin $-\frac{1}{2}$ if the system is in the ground state.

23.4. In an infinite square well of length a there are 5×10^9 electrons per meter. If all the lowest energy levels are filled, determine the energy of the most energetic electron.

Since there are two electrons in each energy level, the total number of electrons up to and including the last or nth level is $N = 2n$. The number of electrons per unit length is therefore

$$\frac{N}{a} = \frac{2n}{a} = 5 \times 10^9\ \text{m}^{-1}$$

so that

$$\frac{n}{a} = (2.5 \times 10^9\ \text{m}^{-1})\left(10^{-10}\ \frac{\text{m}}{\text{Å}}\right) = 0.25\ \text{Å}^{-1}$$

The energy of the nth energy level is thus

$$E_n = \frac{n^2h^2}{8ma^2} = \left(\frac{n}{a}\right)^2 \frac{(hc)^2}{8(mc^2)} = (0.25\ \text{Å}^{-1})^2\,\frac{(12.4 \times 10^3\ \text{eV}\cdot\text{Å})^2}{8(0.511 \times 10^6\ \text{eV})} = 2.35\ \text{eV}$$

23.5. If a nucleus is approximated by a square well, there will be about 1 neutron per 10^{-15} m. In this approximation, determine the energy of the most energetic neutron. The neutron rest mass is 938 MeV.