

**Example 1.1:** Density of Liquid CO<sub>2</sub>

Estimate the density of liquid carbon dioxide based on Figure 1-3.

**Solution** The mean distance between molecules in the liquid is approximately equal to  $r_*$ , the distance where the potential has a minimum. If we imagine molecules to be arranged in a regular cubic lattice at distance  $r_*$  from each other, the volume of  $N_A$  molecules would be  $N_A r_*^3$ . The density of this arrangement is

$$\rho = \frac{M_m}{N_A r_*^3},$$

where  $M_m$  is the molar mass. Using  $r_* = 4.47 \text{ \AA} = 4.47 \times 10^{-10} \text{ m}$ ,  $M_m = 44.01 \times 10^{-3} \text{ kg/mol}$ ,

$$\rho = \frac{44.01 \times 10^{-3} \text{ kg/mol}}{(6.022 \times 10^{23} \text{ mol}^{-1})(4.47 \times 10^{-10} \text{ m})^3} = 818 \text{ kg/m}^3.$$

Perry's *Handbook* (7th ed., Table 2-242) lists the following densities of saturated liquid CO<sub>2</sub> at various temperatures:

$T$ (K)	$\rho$ (kg/m <sup>3</sup> )
216.6	1130.7
270	947.0
300	680.3
304.2	466.2

According to this table, density varies with temperature from 1130.7 kg/m<sup>3</sup> at 216.6 K to 466.2 kg/m<sup>3</sup> at 304.2 K. The calculated value corresponds approximately to 285 K.

**Comments** The calculation based on the intermolecular potential is an estimation. It does not account for the effect of temperature (assumes that the mean distance between molecules is  $r_*$  regardless of temperature) and that molecules are arranged in a regular cubic lattice. Nonetheless, the final result is of the correct order of magnitude, a quite impressive result given the minimal information used in the calculation.

**Ideal-Gas State** Figure 1-3 shows that at distances larger than about 10 Å the potential of carbon dioxide is fairly flat and the molecular force nearly zero. If carbon dioxide is brought to a state such that the mean distance between molecules is more than 10 Å we expect that molecules would hardly register the presence of each other and would largely move independently of each other, except for brief close encounters. This state can be reproduced experimentally by decreasing pressure (increasing volume) while keeping temperature the same. This is called the *ideal-gas state*. It is a *state*—not a gas—and is reached by any gas when pressure is reduced sufficiently. In the ideal-gas state molecules move independently