If we recall that $\omega = (k/m)^{1/2}$, we see that the coefficient of the first term is $kA^2/2$, so that the total energy becomes

$$\begin{aligned} E &= \frac{kA^2}{2}(\sin^2 \omega t + \cos^2 \omega t) \\ &= \frac{kA^2}{2} \end{aligned} \tag{5.15}$$

Thus, we see that the total energy is a constant and, in particular, is equal to the potential energy at its largest displacement, where the kinetic energy is zero. Figure 5.3 shows how the total energy is distributed between the kinetic energy and the potential energy. Each oscillates in time between zero and its maximum value but in such a way that their sum is always a constant. We say that the total energy is conserved and that the system is a *conservative system.*

5–2. The Equation for a Harmonic-Oscillator Model of a Diatomic Molecule Contains the Reduced Mass of the Molecule

The simple harmonic oscillator is a good model for a vibrating diatomic molecule. A diatomic molecule, however, does not look like the system pictured in Figure 5.1 but more like two masses connected by a spring as in Figure 5.4. In this case we have two equations of motion, one for each mass:

$$m_1 \frac{d^2x_1}{dt^2} = k(x_2 - x_1 - l_0) \tag{5.16}$$

and

$$m_2 \frac{d^2x_2}{dt^2} = -k(x_2 - x_1 - l_0) \tag{5.17}$$

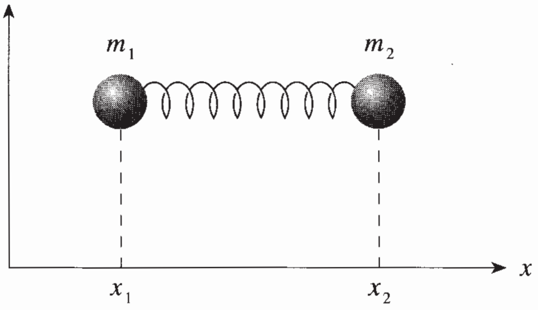

FIGURE 5.4
Two masses connected by a spring, which is a model used to describe the vibrational motion of a diatomic molecule.

where l_0 is the undistorted length of the spring. Note that if $x_2 - x_1 > l_0$, the spring is stretched and the force on mass m_1 is toward the right and that on mass m_2 is toward the left. This is why the force term in Equation 5.16 is positive and that in Equation 5.17 is negative. Note also that the force on m_1 is equal and opposite to the force on m_2, as it should be according to Newton's third law, action and reaction.

If we add Equations 5.16 and 5.17, we find that

$$\frac{d^2}{dt^2}(m_1x_1 + m_2x_2) = 0 \tag{5.18}$$

This form suggests that we introduce a *center-of-mass coordinate*

$$X = \frac{m_1x_1 + m_2x_2}{M} \tag{5.19}$$

where $M = m_1 + m_2$, so that we can write Equation 5.18 in the form

$$M\frac{d^2X}{dt^2} = 0 \tag{5.20}$$

There is no force term here, so Equation 5.20 shows that the center of mass moves uniformly in time with a constant momentum.

The motion of the two-mass or two-body system in Figure 5.4 must depend upon only the *relative* separation of the two masses, or upon the *relative coordinate*

$$x = x_2 - x_1 - l_0 \tag{5.21}$$

If we divide Equation 5.17 by m_2 and then subtract Equation 5.16 divided by m_1 we find that

$$\frac{d^2x_2}{dt^2} - \frac{d^2x_1}{dt^2} = -\frac{k}{m_2}(x_2 - x_1 - l_0) - \frac{k}{m_1}(x_2 - x_1 - l_0)$$

or

$$\frac{d^2}{dt^2}(x_2 - x_1) = -k\left(\frac{1}{m_1} + \frac{1}{m_2}\right)(x_2 - x_1 - l_0)$$

If we let

$$\frac{1}{m_1} + \frac{1}{m_2} = \frac{m_1 + m_2}{m_1m_2} = \frac{1}{\mu}$$

and introduce $x = x_2 - x_1 - l_0$ from Equation 5.21, then we have

$$\mu\frac{d^2x}{dt^2} + kx = 0 \tag{5.22}$$

The quantity μ that we have defined is called the *reduced mass*.

Equation 5.22 is an important result with a nice physical interpretation. If we compare Equation 5.22 with Equation 5.3, we see that Equation 5.22 is the same except for the substitution of the reduced mass μ. Thus, the two-body system in Figure 5.4 can be treated as easily as the one-body problem in Figure 5.1 by using the reduced mass of the two-body system. In particular, the motion of the system is governed by Equation 5.6 but with $\omega = (k/\mu)^{1/2}$. Generally, if the potential energy depends upon only the *relative* distance between two bodies, then we can introduce relative coordinates such as $x_2 - x_1$ and reduce a two-body problem to a one-body problem. This important and useful theorem of classical mechanics is discussed in Problems 5–5 and 5–6.

5–3. The Harmonic-Oscillator Approximation Results from the Expansion of an Internuclear Potential Around its Minimum

Before we discuss the quantum-mechanical treatment of a harmonic oscillator, we should discuss how good an approximation it is for a vibrating diatomic molecule. The internuclear potential for a diatomic molecule is illustrated by the solid line in Figure 5.5. Notice that the curve rises steeply to the left of the minimum, indicating the difficulty of pushing the two nuclei closer together. The curve to the right side of the equilibrium position rises intially but eventually levels off. The potential energy at large separations is essentially the bond energy. The dashed line shows the potential $\frac{1}{2}k(l - l_0)^2$ associated with Hooke's law. Although the harmonic-oscillator potential may appear to be a terrible approximation to the experimental curve, note that it is, indeed, a good approximation in the region of the minimum. This region is the

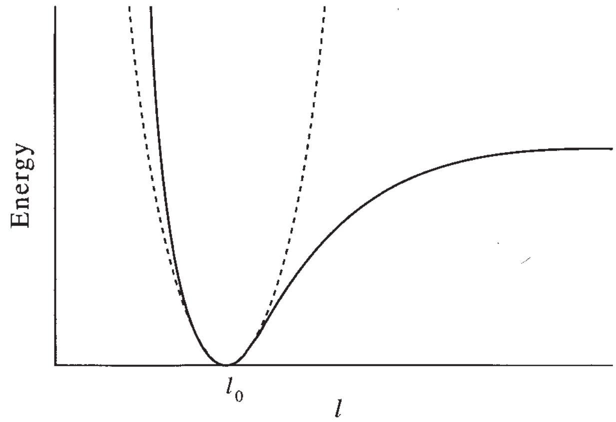

FIGURE 5.5
A comparison of the harmonic oscillator potential ($k(l - l_0)^2/2$; dashed line) with the complete internuclear potential (solid line) of a diatomic molecule. The harmonic oscillator potential is a satisfactory approximation at small displacements.