$V$. Choose $R = 2000\,\Omega$, $C = 10^{-6}$ farads, and $V = 10$ volts. Do you expect $Q(t)$ to increase with $t$? Does $Q(t)$ increase indefinitely, or does it reach a steady-state value? Use a program to solve (4.23) numerically using the Euler algorithm. What value of $\Delta t$ is necessary to obtain three decimal accuracy at $t = 0.005$?

(b) What is the nature of your numerical solution to (4.23) at $t = 0.05$ for $\Delta t = 0.005$, 0.0025, and 0.001? Does a small change in $\Delta t$ lead to a large change in the computed value of $Q$? Is the Euler algorithm stable for reasonable values of $\Delta t$?  ∎

## 4.7 ■ PROJECTS

### Project 4.17  Chemical oscillations

The kinetics of chemical reactions can be modeled by a system of coupled first-order differential equations. As an example, consider the following reaction:

$$A + 2B \rightarrow 3B + C, \tag{4.26}$$

where $A$, $B$, and $C$ represent the concentrations of three different types of molecules. The corresponding rate equations for this reaction are

$$\frac{dA}{dt} = -kAB^2 \tag{4.27a}$$

$$\frac{dB}{dt} = kAB^2 \tag{4.27b}$$

$$\frac{dC}{dt} = kAB^2. \tag{4.27c}$$

The rate at which the reaction proceeds is determined by the reaction constant $k$. The terms on the right-hand side of (4.27) are positive if the concentration of the molecule increases in (4.26) as it does for $B$ and $C$, and negative if the concentration decreases as it does for $A$. Note that the term $2B$ in the reaction (4.26) appears as $B^2$ in the rate equation (4.27). In (4.27) we have assumed that the reactants are well stirred so that there are no spatial inhomogeneities. In Section 7.8 we will discuss the effects of spatial inhomogeneities due to molecular diffusion.

Most chemical reactions proceed to equilibrium, where the mean concentrations of all molecules are constant. However, if the concentrations of some molecules are replenished, it is possible to observe oscillations and chaotic behavior (see Chapter 6). To obtain oscillations, it is essential to have a series of chemical reactions such that the products of some reactions are the reactants of others. In the following, we consider a simple set of reactions that can lead to oscillations under certain conditions (see Lefever and Nicolis):

$$A \rightarrow X \tag{4.28a}$$

$$B + X \rightarrow Y + D \tag{4.28b}$$

$$2X + Y \rightarrow 3X \tag{4.28c}$$

$$X \rightarrow C. \tag{4.28d}$$

If we assume that the reverse reactions are negligible and $A$ and $B$ are held constant by an external source, the corresponding rate equations are

$$\frac{dX}{dt} = A - (B + 1)X + X^2Y \tag{4.29a}$$

$$\frac{dY}{dt} = BX - X^2Y. \tag{4.29b}$$

For simplicity, we have chosen the rate constants to be unity.

(a) The steady state solution of (4.29) can be found by setting $dX/dt$ and $dY/dt$ equal to zero. Show that the steady state values for $(X, Y)$ are $(A, B/A)$.

(b) Write a program to solve numerically the rate equations given by (4.29). Your program should input the initial values of $X$ and $Y$ and the fixed concentrations $A$ and $B$, and plot $X$ versus $Y$ as the reactions evolve.

(c) Systematically vary the initial values of $X$ and $Y$ for given values of $A$ and $B$. Are their steady state behaviors independent of the initial conditions?

(d) Let the initial value of $(X, Y)$ equal $(A + 0.001, B/A)$ for several different values of $A$ and $B$, that is, choose initial values close to the steady state values. Classify which initial values result in steady state behavior (stable) and which ones show periodic behavior (unstable). Find the relation between $A$ and $B$ that separates the two types of behavior.  ∎

### Project 4.18  Nerve impulses

In 1952 Hodgkin and Huxley developed a model of nerve impulses to understand the nerve membrane potential of a giant squid nerve cell. The equations they developed are known as the Hodgkin–Huxley equations. The idea is that a membrane can be treated as a capacitor where $CV = q$, and thus the time rate of change of the membrane potential $V$ is proportional to the current $dq/dt$ flowing through the membrane. This current is due to the pumping of sodium and potassium ions through the membrane, a leakage current, and an external current stimulus. The model is capable of producing single nerve impulses, trains of nerve impulses, and other effects. The model is described by the following first-order differential equations:

$$C\frac{dV}{dt} = -g_K n^4(V - V_K) - g_{Na}m^3h(V - V_{Na}) - g_L(V - V_L) + I_{ext}(t) \tag{4.30a}$$

$$\frac{dn}{dt} = \alpha_n(1 - n) - \beta_n n \tag{4.30b}$$

$$\frac{dm}{dt} = \alpha_m(1 - m) - \beta_m m \tag{4.30c}$$

$$\frac{dh}{dt} = \alpha_h(1 - h) - \beta_h h, \tag{4.30d}$$

where $V$ is the membrane potential in millivolts (mV), $n$, $m$, and $h$ are time dependent functions that describe the gates that pump ions into or out of the cell, $C$ is the membrane capacitance per unit area, the $g_i$ are the conductances per unit area for potassium, sodium,