量子化学作业 第二章 （2017-2018 学期）

2-2. Solve the following differential equations:

$$(a)\frac{d^2y}{dx^2}-4y=0 \qquad y(0)=2 \qquad \frac{dy}{dx}\Big|_{x=0}=4$$

$$(b)\frac{d^2y}{dx^2}-5\frac{dy}{dx}+6y=0 \qquad y(0)=-1 \qquad \frac{dy}{dx}\Big|_{x=0}=0$$

$$(c)\frac{dy}{dx}-2y=0 \qquad y(0)=2$$

2-3. Prove that $x(t)=\cos\omega t$ oscillates with a frequency $\nu=\omega/2\pi$. Prove that $x(t)=A\cos\omega t+B\sin\omega t$ oscillates with the same frequency, $\omega/2\pi$.

2-7. This problem develops the idea of a classical harmonic oscillator. Consider a mass m m attached to a spring, as shown in Figure 2.11. Suppose there is no gravitational force acting on m so that the only force is from the spring. Let the relaxed or undistorted length of the spring be x_0. Hooke's law says that the force acting on the mass m is $f=-k(x-x0)$, where k is a constant characteristic of the spring and is called the force constant of the spring. Note that the minus sign indicates the direction of the force: to the left if $x>x_0$ (extended) and to the right if $x<x_0$ (compressed). The momentum of the mass is:

$$p = m\frac{dx}{dt} = m\frac{d(x-x_0)}{dt}$$

Newton's second law says that the rate of change of momentum is equal to a force:

$$\frac{dp}{dt} = f$$

Replacing $f(x)$ by Hooke's law, show that:s

$$m\frac{d^2x}{dt^2} = -k(x-x_0)$$

Upon letting $\xi = x - x_0$ be the displacement of the spring from its undistorted length, then:

$$m\frac{d^2\xi}{dt^2} + k\xi = 0$$

Given that the mass starts at $\xi = 0$ with an initial velocity v_0, show that the displacement is given by

$$\xi(t) = v_0(\frac{m}{k})^{1/2}\sin[(\frac{k}{m})^{1/2}t]$$

Interpret and discuss this solution. What does the motion look like? What is the frequency? What is the amplitude?

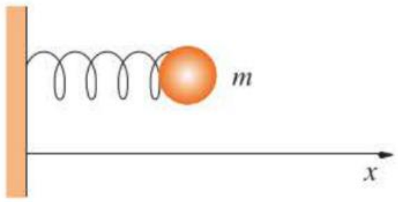

FIGURE 2.11
A body of mass m connected to a wall by a spring.

2-8. Modify Problem 2-7 to the case where the mass is moving through a viscous medium with a viscous force proportional to but opposite the velocity. Show that the equation of motion is:

$$m\frac{d^2\xi}{dt^2}+\gamma\frac{d\xi}{dt}+k\xi=0$$

where γ is the viscous drag coefficient. Solve this equation and discuss the behavior of $\xi(t)$ for various values of m,γ,k. This system is called a damped harmonic oscillator.

2-10. We will see in Chapter 3 that the Schrodinger equation for a particle of mass m that is constrained to move freely along a line between 0 and a is:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}=E\psi \quad (\hbar=h/2\pi)$$

with the boundary condition：

$$\psi(0)=\psi(a)=0$$

In this equation, E is the energy of the particle and $\psi(x)$ is its wave function. Solve this differential equation for $\psi(x)$, apply the boundary conditions, and show that the energy can have only the values:

$$E_n=\frac{\pi^2\hbar^2n^2}{2ma^2} \quad (n=1,2,3...)$$

or that the energy is quantized.

2-17. Prove that $\mu_n(x,t)$, the nth normal mode of a vibrating string (Equation 2.23), can be written as the superposition of two similar traveling waves moving in opposite directions. (Let $\phi_n = 0$ in Equation 2.25.)

B-2. A discrete probability distribution that is commonly used in statistics is the Poisson distribution:

$$f_n = \frac{\lambda^n}{n!} e^{-\lambda} \qquad (n = 0, 1, 2, \ldots)$$

where λ is a positive constant. Prove that f_n is normalized. Evaluate $< n >$ and $< n^2 >$ and show that $\sigma^2 > 0$. Recall that

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!}$$

B-3. An important continuous distribution is the exponential distribution:

$$p(x)dx = ce^{-\lambda x}dx \qquad 0 \le x < \infty$$

Evaluate $c, \langle x \rangle$ and σ^2, and the probability that $x > a$.