Chemistry 331 **Tutorial #2**

1. a) The unit vectors along the x, y and z-directions are $\hat{i}, \hat{j}, \hat{k}$ respectively. If

$$A = \pi\hat{i} + 3\hat{j} - 1\hat{k} \quad \text{and} \quad \mathbf{B} = 2\pi\hat{i} - 3\hat{j} + 7\hat{k}$$

find $A + B$, $A - B$, $3A$, and $-2A$

b) Find the dot product of A and B

c) The length of a vector V defined as $|V| = \sqrt{V \cdot V}$, that is, as the square root of the dot product of the vector V with itself. Find $|A|$ and $|B|$ from part a).

2. a) Find the gradient of the scalar function

$$h(x, y) = \frac{x^{2}y^{2}e^{-y/10}}{10 + 3x}$$

b) Suppose that h is the elevation in meters above sea level of the earth's surface and x and y are distances in kilometers north and east, respectively, from a reference point. What is the direction of steepest descent at $x = 10$ and $y = 20$?

3. In three-dimensional space, a classical particle moves in a potential energy field given by:

$$V(x, y, z) = ax^3 + by^3 + cz^3 + dxy + exz + fyz$$

where a, b, c, d, e, and f are constants.

When the particle is at point $x = 1$ cm, $y = 2$ cm, and $z = 3$ cm, what are the x-, y- and z-components of force acting on it in terms of constants of the problem?

4. Newton's equation of motion for a particle of mass moving freely in the +ve x-direction is:

$$F_x = m\frac{d^2x}{dt^2} = 0$$

a) Find the position as a function of time, $x(t)$, subject to the following initial conditions: position $x = x_o$ and velocity $v = v_o$ at time $t = 0$.

b) What is the momentum of the particle, p_x, as a function of time. *(Note: p_x and x are well determined in classical mechanics, but as we shall see, are not in quantum mechanics).*

5. Newton's equation of motion for a 1-dimensional (x-direction) spring system undergoing simple harmonic motion, with a spring force constant, k, and mass m is given by:

$$F_x = m\frac{d^2x}{dt^2} = -kx$$

A solution of this differential equation is $x = x_0\cos(\omega t)$ with the angular frequency of oscillation

$$\omega = \sqrt{\frac{k}{m}}$$

A block of mass $m = 0.50$ kg connected to a spring motion oscillates with a peak amplitude of $x_0 = 35$ cm and the motion is repeated every 0.5 s.

Find the

a) period
b) frequency in Hz
c) angular frequency in radians per second
d) spring force constant k
e) maximum speed of the block
f) maximum force exerted on the block.

6. *Where does Schrodinger's famous wave equation come from?*

a) Convince yourself that

$$\Psi(x,t) = A\sin\left(\frac{2\pi x}{\lambda}\right)\cos\left(\frac{2\pi \mathrm{v}t}{\lambda}\right)$$

is a wave of amplitude A, wavelength λ and frequency ν traveling in the x-direction with velocity $\mathrm{v} = \nu\lambda$.

b) Prove that $u(x, t)$ is a solution of the classical wave equation

$$\left(\frac{\partial^2 u}{\partial t^2}\right)_x = \mathrm{v}^2\left(\frac{\partial^2 u}{\partial x^2}\right)_t$$

c) Illustrating "separation of variables", notice that $u(x, t)$ is a product of functions that depend on x or t, but not both. The time-dependent factor can be expressed as $\cos(2\pi \mathrm{v}t/\lambda)$ and the spatial factor is $\psi(x) = A\sin(2\pi x/\lambda)$. Substitute the expression for $u(x, t)$ into the classical wave equation

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(1.) a) $\vec{A} = \pi\hat{i} + 3\hat{j} - 1\hat{k}$ $\quad\quad$ $\vec{B} = 2\pi\hat{i} - 3\hat{j} + 7\hat{k}$

$$\vec{A}+\vec{B} = (\pi+2\pi)\hat{i} + (3-3)\hat{j} + (-1+7)\hat{k} = 3\pi\hat{i} + 6\hat{k}$$

$$\vec{A}-\vec{B} = (\pi-2\pi)\hat{i} + (3-(-3))\hat{j} + (-1-7)\hat{k} = -\pi\hat{i} + 6\hat{j} - 8\hat{k}$$

$$3\vec{A} = 3\pi\hat{i} + 9\hat{j} - 3\hat{k} \qquad -2\vec{A} = -2\pi\hat{i} - 6\hat{j} + 2\hat{k}$$

b) $$\vec{A}\cdot\vec{B} = \pi(2\pi) + 3(-3) + (-1)(7) = 2\pi^2 - 9 - 7 = 2\pi^2 - 16$$
$$= 3.7392\ldots$$

c) $$|A| = \sqrt{\pi^2 + 3^2 + 1^2} = \sqrt{\pi^2 + 10} = 4.4575\ldots$$
$$|B| = \sqrt{(2\pi)^2 + (-3)^2 + 7^2} = \sqrt{4\pi^2 + 58} = 9.8731\ldots$$
$$\vec{A}\cdot\vec{B} = |\vec{A}||\vec{B}|\cos\theta \qquad \cos\theta = \frac{3.7392\ldots}{44.0097\ldots} = 0.08496\ldots$$
$$\theta = 85.13\ldots^\circ = 1.485\ldots \text{ radians}$$

(2.) $$h = \frac{x^2 y^2 e^{-y/10}}{10+3x} \qquad \text{gradient } \vec{\nabla} h = \frac{\partial h}{\partial x}\hat{i} + \frac{\partial h}{\partial y}\hat{j}$$

$$\frac{\partial h}{\partial x} = \left(\frac{\partial}{\partial x}\frac{x^2 y^2 e^{-y/10}}{10+3x}\right)_y = y^2 e^{-y/10}\frac{\partial}{\partial x}\left(\frac{x^2}{10+3x}\right) \quad \text{at } (y \text{ constant})$$

$$= y^2 e^{-y/10}\frac{(10+3x)2x - x^2 3}{(10+3x)^2} = y^2 e^{-y/10}\frac{x(20+6x-3x)}{(10+3x)^2}$$

$$\frac{\partial h}{\partial x} = \frac{x(20+3x)\, y^2 e^{-y/10}}{(10+3x)^2}$$

$$\frac{\partial h}{\partial y} = \left(\frac{\partial}{\partial y}\frac{x^2 y^2 e^{-y/10}}{10+3x}\right)_x = \frac{x^2}{10+3x}\frac{\partial (y^2 e^{-y/10})}{\partial y}$$

$$= \frac{x^2}{10+3x}\left(-\frac{y^2}{10}e^{-y/10} + 2y\, e^{-y/10}\right) = \frac{x^2 y\left(2 - \frac{y}{10}\right)e^{-y/10}}{10+3x}$$

(2 a) cont.)

$$\vec{\nabla} h = \frac{\partial h}{\partial x}\hat{\imath} + \frac{\partial h}{\partial y}\hat{\jmath} = \frac{x(20+3x)y^2 e^{-y/10}}{(10+3x)^2}\hat{\imath} + \frac{x^2 y(2-\frac{y}{10})e^{-y/10}}{10+3x}\hat{\jmath}$$

b) $x = 10 \qquad y = 20$

$$\vec{\nabla} h = \frac{10(20+30)\,20^2 e^{-2}}{(10+30)^2}\hat{\imath} + \frac{10^2(20)(2-2)e^{-2}}{10+30}\hat{\jmath}$$

$$= 125 e^{-2}\,\hat{\imath} + (0)\hat{\jmath} = 16.92\,\hat{\imath}$$

the slope in the x-direction (north) is 16.92
the slope in the y-direction (east) is 0

steepest descent: move due south

(3.) potential energy $V(x,y,z) = ax^3 + by^3 + cz^3 + dxy + exz + fyz$

force $\vec{F} = -\vec{\nabla} V$ (negative gradient of the potential energy)

$$\vec{F}(x,y,z) = -\frac{\partial V}{\partial x}\hat{\imath} - \frac{\partial V}{\partial y}\hat{\jmath} - \frac{\partial V}{\partial z}\hat{k}$$

$$= -(3ax^2 + dy + ez)\hat{\imath} - (3by^2 + dx + fz)\hat{\jmath} - (3cz^2 + ex + fy)\hat{k}$$

$$= -(3a1^2 + d2 + e3)\hat{\imath} - (3b4 + d(1) + f3)\hat{\jmath} - (3c9 + e + f2)\hat{k}$$

$$= -(3a + 2d + 3e)\hat{\imath} - (12b + d + 3f)\hat{\jmath} - (27c + e + 2f)\hat{k}$$

4. for a particle of mass m moving freely (no forces acting on it) in the x-direction

$$F_x = 0 = m\frac{d^2x}{dt^2} \left(= m\frac{d}{dt}\left(\frac{dx}{dt}\right) = m\frac{dv}{dt} \right)$$

a)

the acceleration dv/dt is zero (constant velocity)

the n-th derivative of a polynomial of degree n-1 is zero

so $x = c_1 + c_2 t$ $\quad c_1, c_2$ are constants

at $t=0$, $x = x_0 = c_1 + c_2(0) = c_1$

$t = 0$, $v = v_0 = \left.\frac{dx}{dt}\right|_{t=0} = c_2$

$c_1 = x_0$
$c_2 = v_0$

$$x(t) = x_0 + v_0 t$$

b) $p_x(t) = m v_x(t) = m c_2$

5. $F_x = m\frac{d^2x}{dt^2} = -kx$

the force is proportional to the distance x and acts in the opposite direction (restoring force)

$$x(t) = x_0 \cos(\omega t)$$

$$\frac{dx}{dt} = -x_0\omega \sin(\omega t) \qquad \frac{d^2x}{dt} = -x_0\omega\frac{d}{dt}(\sin\omega t) = -x_0\omega^2\cos\omega t$$

$$m\frac{d^2x}{dt^2} = -kx = -k x_0 \cos\omega t = -m x_0 \omega^2 \cos\omega t$$

$$\omega^2 = k/m \qquad \omega = \sqrt{k/m}$$

$x = x_0 \cos\left(\sqrt{\frac{k}{m}}\, t\right)$ $\qquad x_0 = 35 \text{ cm}$ (given)

a) repeat motion every 0.5 s $\qquad$ period = 0.5 s (given)

b) frequency is one oscillation per 0.5 s = 2 oscillations per second

$= 2 \text{ Hz} = \nu = 2 s^{-1}$

c) one oscillation = 2π radians

ω = angular frequency $= \dfrac{2\pi}{0.5 \text{ sec}} = 4\pi s^{-1} = 2\pi\nu$

d) $k = m\omega^2 = 0.50 \text{ kg} (4\pi s^{-1})^2 = 8\pi^2 \text{ kg } s^{-2}$

$= 78.96 \text{ kg } s^{-2} = 78.96 \ \dfrac{N}{m}$

e) $v = \dfrac{dx}{dt} = -x_0 \omega \sin(\omega t)$ $\qquad -1 \le \sin(\omega t) \le 1$

$\therefore$ max v when $\sin \omega t = 1$ $\qquad v_{max} = -x_0\omega(-1) = x_0\omega$

$v_{max} = (35 \text{ cm})(4\pi s^{-1}) = 439.8 \text{ cm } s^{-1}$

f) force $= m\dfrac{d^2x}{dt^2} = -m x_0 \omega^2 \cos\omega t$

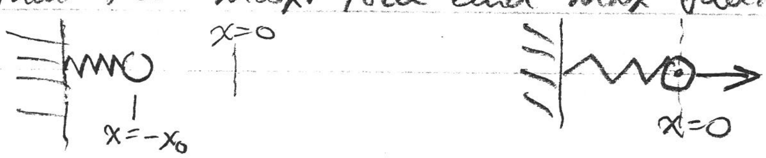
$-1 \le \cos\omega t \le 1$

max force when $\cos(\omega t) = -1$ $\qquad F_{x\,max} = m x_0 \omega^2$

$F_{x\,max} = (0.50 \text{ kg})(0.35 \text{ m})(4\pi s^{-1})^2 = 27.63 \text{ N}$

notice that the max. force and max velocity are 180° out of phase

v = 0
max F



F = 0
max V

6 a) $\psi(x,t) = A \sin\left(\frac{2\pi x}{\lambda}\right) \cos\left(\frac{2\pi v t}{\lambda}\right)$

notice that $\sin\left(\frac{2\pi x}{\lambda}\right)$ completes one complete cycle

0 to 2π, 2π to 4π, 4π to 6π, etc when

$\frac{x}{\lambda}$ changes from 0 to 1, 1 to 2, 2 to 3, etc.

λ is clearly the wavelength
for a wave travelling with velocity v:

b) $$\frac{\partial \psi}{\partial t} = -A \sin\left(\frac{2\pi x}{\lambda}\right)\left(\frac{2\pi v}{\lambda}\right)\sin\left(\frac{2\pi v t}{\lambda}\right)$$

$$\frac{\partial^2 \psi}{\partial t^2} = -A \sin\left(\frac{2\pi x}{\lambda}\right)\left(\frac{2\pi v}{\lambda}\right)^2 \cos\left(\frac{2\pi v t}{\lambda}\right) = -\left(\frac{2\pi v}{\lambda}\right)^2 \psi(x,t)$$

$$\frac{\partial \psi}{\partial x} = A \frac{2\pi}{\lambda} \cos\left(\frac{2\pi x}{\lambda}\right) \cos\left(\frac{2\pi v t}{\lambda}\right)$$

$$\frac{\partial^2 \psi}{\partial x^2} = A\left(\frac{2\pi}{\lambda}\right)^2 \sin\left(\frac{2\pi x}{\lambda}\right) \cos\left(\frac{2\pi v t}{\lambda}\right) = -\left(\frac{2\pi}{\lambda}\right)^2 \psi(x,t)$$

so $$\frac{\partial^2 \psi}{\partial t^2} = v^2 \frac{\partial^2 \psi}{\partial x^2}$$

c) $$\frac{\partial^2 \psi}{\partial t^2} = -A \sin\left(\frac{2\pi x}{\lambda}\right)\left(\frac{2\pi v}{\lambda^2}\right)^2 \cos\left(\frac{2\pi v t}{\lambda}\right) = v^2 \frac{\partial^2 \psi}{\partial x^2}$$

$$= v^2\left[\frac{\partial^2}{\partial x^2}\left(A \sin\left(\frac{2\pi x}{\lambda}\right)\cos\left(\frac{2\pi v t}{\lambda}\right)\right)\right]$$

$$\overbrace{-A \sin\left(\frac{2\pi x}{\lambda}\right)}^{\psi(x)}\left(\frac{2\pi v}{\lambda}\right)^2 \cancel{\cos\left(\frac{2\pi v t}{\lambda}\right)} = \cancel{v^2} \cancel{\cos\left(\frac{2\pi v t}{\lambda}\right)} \frac{d^2}{dx^2}\left[A \sin\left(\frac{2\pi x}{\lambda}\right)\right]$$

(6c cont.) $-\left(\frac{2\pi}{\lambda}\right)^2 \psi(x) = \frac{d^2\psi(x)}{dx^2}$

or $\frac{d^2\psi(x)}{dx^2} + \left(\frac{2\pi}{\lambda}\right)^2 = 0$

$E = \frac{1}{2}mv^2 = \frac{(mv)^2}{2m} = \frac{p^2}{2m}$

d) $\frac{1}{\lambda} = \frac{p}{h}$ $\frac{1}{\lambda^2} = \frac{p^2}{h^2} = \frac{2mE}{h^2}$

$0 = \frac{d^2\psi(x)}{dx^2} + \left(\frac{2\pi}{\lambda}\right)^2 \psi(x) = \frac{d^2\psi(x)}{dx^2} + \frac{(2\pi)^2 2mE}{h^2}\psi(x) = \frac{d^2\psi(x)}{dx^2} + \frac{8\pi^2 mE}{h^2}\psi(x)$

e) The general solution to $\frac{d^2\psi(x)}{dx^2} + \frac{8\pi^2 mE}{h^2}\psi(x) = 0$

(a second-order differential equation indicating that the second derivative gives the function times a negative constant)

is $\psi(x) = c_1 \sin kx + c_2 \cos(kx)$

if $\psi(0) = 0$, then $c_2 = 0$
(given) furthermore
if $\psi(a) = 0$, then $ka = \pi, 2\pi, 3\pi, \ldots$
or $ka = n\pi$ $k = \frac{n\pi}{a}$

$\frac{d^2\psi(x)}{dx^2} = -c_1 k^2 \sin kx = -\frac{8\pi^2 mE}{h^2} c_1 \sin kx$

$k^2 = \frac{8\pi^2 mE}{h^2}$ $E = \frac{h^2 k^2}{8\pi^2 m} = \frac{h^2 n^2 \pi^2}{8\pi^2 m a^2} = \frac{h^2}{8ma^2} n^2$