3.012 Fund of Mat Sci: Bonding – Lecture 1 bis

WAVE MECHANICS

Photo courtesy of Malene Thyssen, www.mtfoto.dk/malene/

Last Time

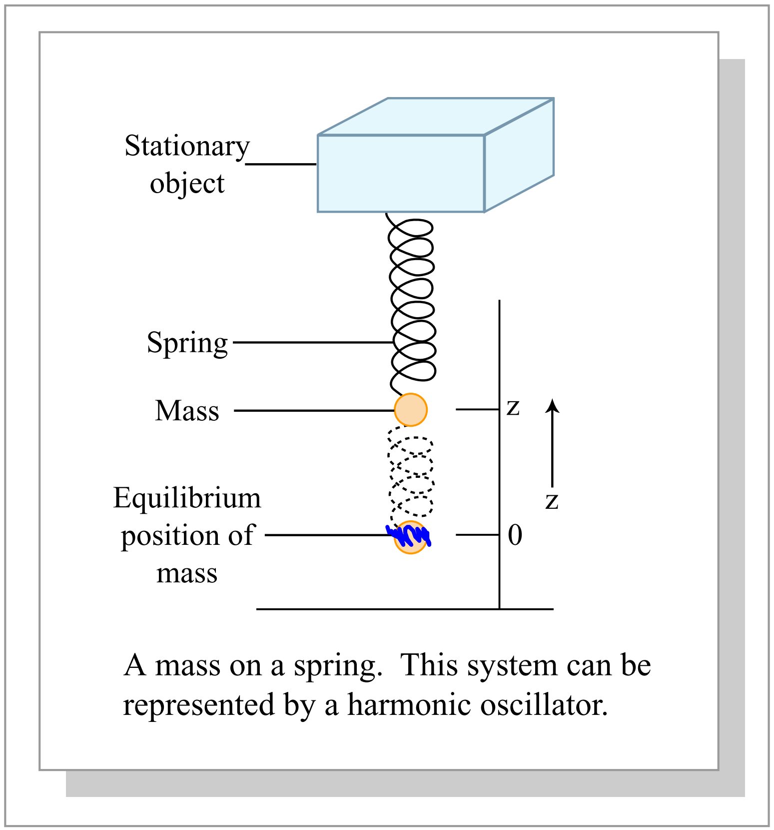
1. Players: particles (protons and neutrons in the nuclei, electrons) and electromagnetic fields (photons)
2. Forces: electromagnetic
3. Dynamics: Newton (macroscopic), Maxwell (fields), Schrödinger (microscopic)
4. De Broglie relation $\lambda \bullet p = h$

Homework for Mon 12

- You know by now: 12.5, 13.2, 13.3
- Study: 13.4 and 13.5

•Notes on harmonic oscillator -- Section 14.1 in Mortimer, R. G. *Physical Chemistry*. 2nd ed. San Diego, CA: Elsevier, 2000.

Harmonic Oscillator (I)



A mass on a spring. This system can be represented by a harmonic oscillator.

Figure by MIT OCW.

$$V(z) = V(0) + \alpha z + \frac{1}{2} k z^2 + \ldots$$

$$\vec{F} = -\vec{\nabla} V(z) \Rightarrow F = -\frac{dV(z)}{dz}$$

$$F = -\alpha - kz \ldots \Rightarrow \alpha = 0$$

$F = -kz$ HOOKE'S LAW

Harmonic Oscillator (II)

$$F = ma \implies -kz = m \frac{d^2 z}{dt^2}$$

$$\frac{d^2 z(t)}{dt^2} = -\frac{k}{m} z(t)$$

$$\sin(\omega t)$$

$$\omega \cos(\omega t)$$

$$(-\omega)\,\omega \sin(\omega t)$$

$$\sin(\omega t)$$

$$\cos(\omega t)$$

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

Harmonic Oscillator (III)

Graph of the behavior of a harmonic oscillator removed for copyright reasons.

See Mortimer, R. G. *Physical Chemistry*. 2nd ed. San Diego, CA: Elsevier, 2000, p. 495, figure 14.2.

$$z(t) = A \sin(\omega t) + B \cos(\omega t)$$

$$z(t=0) = z_0$$

$$v(t=0) = \left.\frac{dz(t)}{dt}\right|_{t=0} = 0$$

$$z(t=0) = B = z_0$$

$$z' = \frac{dz}{dt} = A\omega \cos \omega t - B\omega \sin \omega t$$

$$\Rightarrow A\omega = 0$$

The total energy of the system

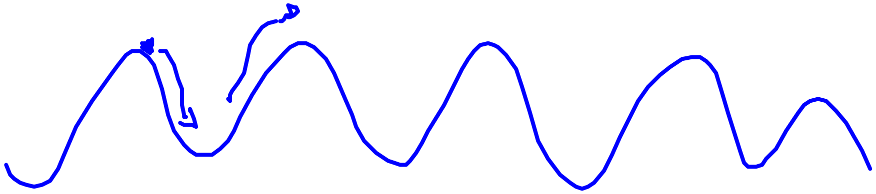
- Kinetic energy K

$$K = \frac{1}{2} m v^2$$

- Potential energy V

$$V(z) = -kz$$

$$\Rightarrow K + V = \text{CONSTANT}$$



Polar Representation

$$z = (3.2, 1.8)$$

Diagram of the Argand plane removed for copyright reasons.

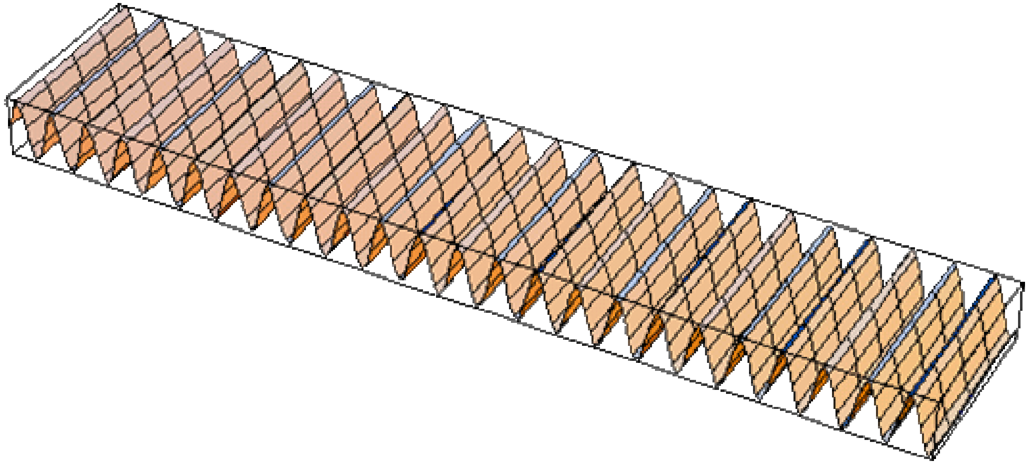
See Mortimer, R. G. *Physical Chemistry*. 2nd ed.
San Diego, CA: Elsevier, 2000, p. 1011, figure B.6.

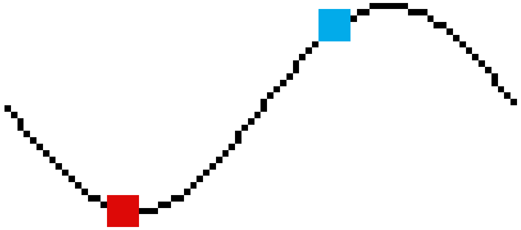
$$e^{i\varphi} = \cos\varphi + i\sin\varphi$$

$$(\cos\varphi, \sin\varphi) = e^{i\varphi}$$

A Traveling "Plane" Wave

$$\Psi(\vec{r},t) = A\exp[i(\vec{k}\cdot\vec{r} - \omega t)]$$





Principle of Linear Superposition

Photo courtesy of Spiralz

Wave-particle Duality

- *Waves have particle-like properties:*
  - *Photoelectric effect: quanta (photons) are exchanged discretely*
  - *Energy spectrum of an incandescent body looks like a gas of very hot particles*

Diagrams of the photoelectric effect and of a P-N solar cell, removed for copyright reasons.

Wave-particle Duality

- Particles have wave-like properties:
  - Electrons in an atom act like standing waves (harmonics) in an organ pipe
  - Electrons beams can be diffracted, and we can see the fringes (Davisson and Germer, at Bell Labs in 1926…)

When is a particle like a wave ?

Wavelength • momentum = Planck

Image of the double-slit experiment removed for copyright reasons.

See the simulation at http://www.kfunigraz.ac.at/imawww/vqm/movies.html:

"Samples from *Visual Quantum Mechanics*": "Double-slit Experiment."

↕

$$\lambda \bullet p = h$$

$$(h = 6.626 \times 10^{-34} \text{ J s} = 2\pi \text{ a.u.})$$

See animation at http://www.kfunigraz.ac.at/imawww/vqm/movies.html
Select "Samples from *Visual Quantum Mechanics*" > "Double-slit experiment"

Time-dependent Schrödinger's equation

(Newton's 2nd law for quantum objects)

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r},t)+V(\vec{r},t)\Psi(\vec{r},t)=i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t}$$

1925-onwards: E. Schrödinger (wave equation), W. Heisenberg (matrix formulation), P.A.M. Dirac (relativistic)

Plane waves as free particles

Our free particle $\Psi(\vec{r},t) = A\exp[i(\vec{k}\cdot\vec{r} - \omega t)]$ satisfies the wave equation:

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r},t) = i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t}$$

(provided $E = \hbar\omega = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$)

Stationary Schrödinger's Equation (I)

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r},t)+V(\vec{r},t)\Psi(\vec{r},t)=i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t}$$

Stationary Schrödinger's Equation (II)

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\varphi(\vec{r}) = E\varphi(\vec{r})$$