3.024 Electrical, Optical, and Magnetic Properties of Materials
Recitation 2 Notes

Outline

1. Hamiltonian Mechanics Review
2. Taylor Series Review & Hyperbolic Function Review
3. Wave-Particle Duality

1. Hamiltonian Mechanics Review

$$H = T + V = E$$

The Hamiltonian H for cases we will examine is the total energy E.
For classical systems, if H is known, the time evolution of the system can be obtained by solving Hamilton's equations:

$$\dot{x}_i = \frac{\partial H}{\partial p_i}$$

$$\dot{p}_i = -\frac{\partial H}{\partial x_i}$$

e.g. 1:
Consider a system with the following Hamiltonian for a single particle in a potential $U(x)$ caused by the surrounding material. Find its equations of motion and solve them for $N = 1$ and $N = 2$ for the time evolution of the system.

$$H = \frac{p^2}{2m} + U(x)$$

$$U(x) = m\omega^2 x^N/N$$

Here ω is a constant and m is the mass of the particle.
We first write Hamilton's equations for this system.

$$\dot{x} = \frac{\partial H}{\partial p} = p/m$$

$$\dot{p} = -\frac{\partial H}{\partial x} = -\frac{\partial U}{\partial x} = -m\omega^2 x^{N-1}$$

Next we combine these equations to obtain a single 2^{nd} order ordinary differential equation.

$$\dot{x} = p/m \rightarrow \dot{p} = m\ddot{x} = -m\omega^2 x^{N-1}$$

For $N = 1$, $\ddot{x}$ is equal to a constant and can be integrated in time t twice to find the solution.

$$\ddot{x} = -\omega^2 \rightarrow \dot{x} = v_0 - \omega^2 t \rightarrow x = x_0 + v_0 t - \omega^2 t^2/2$$

Here x_0 and v_0 are the initial position and velocity of the particle respectively.
For $N = 2$, the system is a 2^{nd} order linear ordinary differential equation.

$$\ddot{x} = -\omega^2 x \rightarrow \ddot{x} + \omega^2 x = 0$$

By inspection we can see this kind of equation has a general solution given as

$$x = A^* e^{-i\omega t} + B^* e^{i\omega t}$$

or equivocally

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

using Euler's equation

$$e^{\pm i\omega t} = \cos(\omega t) \pm i\sin(\omega t)$$

and relations between the integration constants A, B, A^*, and B^*.
Using initial conditions x_0 and v_0, the final general solution in terms of trigonometric functions is

$$x = \frac{x_0 - v_0/\omega}{2}\cos(\omega t) + \frac{x_0 + v_0/\omega}{2}\sin(\omega t)$$

e.g. 2:
N Component system with known energy function.
Consider *N* masses each with a different mass m_i inside a special material. The Hamiltonian of the system in terms of the position and momenta of the particles is given by the following:

$$H = \sum_{i}^{N}\left(\frac{p_i^2}{2m_i} - \sum_{j\neq i}^{N}\frac{m_j g_j (x_i - x_j)^2}{2}\right)$$

Here g_j is a constant characteristic of each mass. Find the equations of motion of this system and solve them for the case $N = 2$.

We first write Hamilton's equations for this system.

$$\dot{x}_i = \frac{\partial H}{\partial p_i} = \frac{p_i}{m_i}$$

$$\dot{p}_i = -\frac{\partial H}{\partial x_i} = \sum_{j\neq i}^{N} m_j g_j (x_i - x_j)$$

Next we combine these equations to obtain a single 2nd order ordinary differential equation.

$$\dot{x}_i = p_i/m_i \rightarrow \dot{p}_i = m_i\ddot{x}_i = \sum_{j\neq i}^{N} m_j g_j (x_i - x_j) = x_i \sum_{j\neq i}^{N} m_j g_j - \sum_{j\neq i}^{N} m_j g_j\, x_j$$

This is actually a matrix equation. Let's consider the matrix form for $N = 2$.

$$\begin{bmatrix} m_1\ddot{x}_1 \\ m_2\ddot{x}_2 \end{bmatrix} = \begin{bmatrix} m_2 g_2 & -m_2 g_2 \\ -m_1 g_1 & m_1 g_1 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

This appears to be a 2nd order linear set of ordinary differential equations. Assume a solution of the form:

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} A_1 \\ A_2 \end{bmatrix} e^{i\omega t}$$

Upon substitution:

$$-\omega^2 \begin{bmatrix} A_1 \\ A_2 \end{bmatrix} e^{i\omega t} = \begin{bmatrix} m_2 g_2 & -m_2 g_2 \\ -m_1 g_1 & m_1 g_1 \end{bmatrix}\begin{bmatrix} A_1 \\ A_2 \end{bmatrix} e^{i\omega t}$$

This is just an eigenvalue problem with omega as the eigenvectors.

$$det\begin{vmatrix} m_2 g_2 + \omega^2 & -m_2 g_2 \\ -m_1 g_1 & m_1 g_1 + \omega^2 \end{vmatrix} = 0$$

$$(m_2 g_2 + \omega^2)(m_1 g_1 + \omega^2) - m_1 g_1 m_2 g_2 = 0$$

$$m_1 g_1 m_2 g_2 + m_1 g_1 \omega^2 + m_2 g_2 \omega^2 + \omega^4 - m_1 g_1 m_2 g_2 = 0$$

$$\omega^2(m_1 g_1 + m_2 g_2 + \omega^2) = 0$$

Therefore there are two eigenvalues:

$$\omega = 0 \text{ and } \omega = \pm i\sqrt{m_1 g_1 + m_2 g_2}$$

The corresponding eigenvectors are found as follows:

$$\text{For } \omega = 0: m_2 g_2 A_1 - m_1 g_1 A_2 = 0 \rightarrow A_1 = \frac{m_1 g_1 A_2}{m_2 g_2}$$

$$\rightarrow \vec{v}_0 = A_2 \begin{bmatrix} \frac{m_1 g_1}{m_2 g_2} \\ 1 \end{bmatrix} \rightarrow \vec{v}_0 = A^* \begin{bmatrix} m_1 g_1 \\ m_2 g_2 \end{bmatrix} \text{ where } A^* = A_2/m_2 g_2 .$$

$$\text{For } \omega = \pm i\sqrt{m_1 g_1 + m_2 g_2}: \; -m_1 g_1 A_1 - m_1 g_1 A_2 = 0 \rightarrow A_1 = -A_2$$

$$\rightarrow \vec{v}_\pm = A_2 \begin{bmatrix} -1 \\ 1 \end{bmatrix} \rightarrow \vec{v}_0 = B^* \begin{bmatrix} 1 \\ -1 \end{bmatrix} \text{ where } B^* = -A_2 .$$

The general solution for $N = 2$ is therefore:

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = A^* \begin{bmatrix} m_1 g_1 \\ m_2 g_2 \end{bmatrix} + B^* \begin{bmatrix} 1 \\ -1 \end{bmatrix} e^{\pm\sqrt{m_1 g_1 + m_2 g_2}t}$$

2. Taylor Series Review

Any function that is infinitely differentiable around a value $x = a$ can be written as a Taylor Series such that:

$$f(x) = \sum_{n=0}^{\infty} \frac{(x-a)^n f^n(a)}{n!}$$

Here $f^n(a)$ represents the nth derivative of the function $f(x)$ evaluated at $x = a$. Taylor Series are useful at approximating transcendental functions around $x = a$ in certain limits by taking a few terms of the Taylor series expansion.

e.g. 3: Fluctuating Charged Particle

The energy of a charged particle fluctuating periodically around another particle it is attached to by a special rod in a downward constant electric field E with length l, mass m, and charge q (positive charge) in terms of its normal coordinate θ is given as:

$$H = \frac{p_\theta^2}{2m} + (mg + qE)l(1 - \cos\theta)$$

Find the equations of motion for this system and solve them in the limit of small θ.

Since we know the Hamiltonian as a function of momenta and coordinates, we can just use Hamilton's equations to find the equations of motion.

$$\dot{\theta} = \frac{\partial H}{\partial p_{\theta_1}} = \frac{p_\theta}{m}$$

$$\dot{p}_{\theta_1} = -\frac{\partial H}{\partial \theta_1} = -(mg - qE)l(\sin\theta)$$

Now, to examine the small angle limits, we will take the Taylor series approximation for sine to first order about $x = 0$.

$$\sin x \cong \frac{(x-0)^0 \sin 0}{0!} + \frac{(x-0)^1 \cos 0}{1!} \rightarrow \sin x \cong x$$

This means to first order the equations of motion reduce to the following:

$$\ddot{\theta} \cong -\left(g + \frac{qE}{m}\right) l\theta$$

This is now simply a first order linear differential equation with exponential general solutions.

$$-\omega^2 e^{-i\omega t} = -\left(g + \frac{qE}{m}\right) l e^{-i\omega t} \to \omega^2 = \left(g + \frac{qE}{m}\right) l$$

Assuming q is positive, the particle for small θ will oscillate with a frequency

$$\omega = \pm\sqrt{\left(g + \frac{qE}{m}\right) l}$$

$$\theta(t) = Ae^{-i\omega t} + Be^{i\omega t}$$

Initial conditions:

$$\theta(0) = \theta_0 \quad \text{and} \quad \dot{\theta}(0) = \psi_0$$

$$A + B = \theta_0 \text{ and } B - A = \frac{\psi_0}{i\omega}$$

$$2A = \theta_0 + \frac{\psi_0}{\omega} e^{\frac{i\pi}{2}} \quad \text{and} \quad 2B = \theta_0 - \frac{\psi_0}{\omega} e^{\frac{i\pi}{2}}$$

$$\theta(t) = \frac{1}{2}\left(\theta_0 e^{-i\omega t} + \frac{\psi_0}{\omega} e^{i\left(\frac{\pi}{2} - \omega t\right)} + \theta_0 e^{i\omega t} - \frac{\psi_0}{\omega} e^{i\left(\frac{\pi}{2} + \omega t\right)}\right)$$

Or in terms of real functions:

$$\theta(t) = \theta_0 \cos \omega t + \frac{\psi_0}{\omega} \sin \omega t$$

Review of hyperbolic functions:

$$\sinh(x) = \frac{e^x - e^{-x}}{2}$$

$$\cosh(x) = \frac{e^x + e^{-x}}{2}$$

$$\tanh(x) = \frac{\sinh(x)}{\cosh(x)}$$

Similarly:

$$\sin(x) = \frac{e^{ix} - e^{-ix}}{2i}$$

$$\cos(x) = \frac{e^{ix} + e^{-ix}}{2}$$

3. Wave-Particle Duality

As seen in lecture, particles such as electrons, protons, neutrons, and even buckyballs (C_{60} fullerenes) all can exhibit wavelike behavior in addition to their normal particle like behavior. Additionally, waves such as light and sound can exhibit particle like behavior.

Key concepts:

The energy of a nonrelativistic particle (speeds << c) is $E = \frac{p^2}{2m}$ with momentum $p = mv$

Massless waves like light have energy based on their wavelength $E = \hbar\omega = h\nu$ with momentum $p = \hbar k = \frac{h}{\lambda}$
Anything with mass can have wavelike behavior based on equating its momentum with its wave vector k which is known as its De Broglie wavelength: $p = mv = \hbar k = \frac{h}{\lambda}$
Likewise, any massless wave can exhibit particle like behavior such that a photon has an effective mass $m = \frac{h}{c\lambda}$ (note this effective mass is just that, an effective mass, photons still have 0 rest mass).

To get a sense of wave-particle duality, consider the following examples:

e.g. 4
A buckyball is composed of 60 carbon atoms in a soccer ball arrangement. At what speed would a buckyball have to be accelerated before wavelike behavior is observed.

Consider wavelike behavior occurs when the De Broglie wavelength is the same as the diameter of the buckyball. The nucleus to nucleus diameter of C_{60} is $d_{C_{60}} \cong 0.71$ nm. The total mass of C_{60} is $m = 60 \cdot 6(1.673 + 1.675)\text{x}10^{-27}$ kg $= 1.205\text{x}10^{-24}$ kg assuming all the carbon atoms are C^{12} isotopes and that the electron mass is negligible.

Then, the velocity the buckyball must travel at is

$$v = \frac{h}{m\lambda} = \frac{6.626 \cdot 10^{-34}\ \mathrm{J \cdot s}}{(1.205 \cdot 10^{-24}\ \mathrm{kg})(0.71 \cdot 10^{-9}\ \mathrm{m})} = 0.7745\,\frac{\mathrm{m}}{\mathrm{s}}$$

Thus, even for such a large object, only small speeds are required to observe wave-particle duality and experimentally interference patterns of beams of buckyballs have been observed.

e.g. 5
What is the De Broglie wavelength of a baseball through by a MLB Red Sox pitcher (v~45 m/s m~0.15 kg).

$$\lambda = \frac{h}{mv} = \frac{6.626 \cdot 10^{-34}\ \mathrm{J \cdot s}}{(0.15\ \ \mathrm{kg})(45\,\frac{\mathrm{m}}{\mathrm{s}})} = 9.8 \cdot 10^{-35}\ \mathrm{m}$$

So a baseball would almost never exhibit wavelike properties when pitched so the batter should not be worrying about the ball interfering with the bat.