

Review of Classical Mechanics

Quantum mechanics is in many ways the accumulation of many hundreds of years of work and thought about how mechanical things move and behave. Since ancient times, scientists have wondered about the structure of matter and have tried to develop a generalized and underlying theory which governs how matter moves at all length scales. For ordinary objects, the rules of motion are very simple. Almost everything we can see and touch and hold conform the classical laws of motion. Classical mechanics is an extremely well developed area of physics. While we may think that classical mechanics has been studied extensively for hundreds of years there really is little new development in this field, it remains an extremely active area of research. Classical mechanics is the workhorse for atomistic simulations of fluids, proteins, polymers. It provides the basis for understanding chaotic systems. It also provides a useful foundation of many of the concepts in quantum mechanics.

Quantum mechanics provides a description of how matter behaves at very small length and mass scales: i.e. in the scale of atoms, molecules, or below them. It was developed over the last century to explain a series of experiments on atomic systems that could not be explained using purely classical treatments. The advent of quantum mechanics forced us to look beyond the classical theories. However, it was not a drastic and complete departure. At some point, the two theories must correspond so that classical mechanics is the limiting behavior of quantum mechanics for macroscopic objects. Consequently, many of the concepts we will study in quantum mechanics have direct analogs to classical mechanics: momentum, angular momentum, time, potential energy, kinetic energy, and action.

Much like classical music is in a particular style, classical mechanics is based upon the principle that the motion of a body can be reduced to the motion of a point particle with a given mass m , position x , and velocity v . In this chapter, we will review some of the concepts of classical mechanics which are necessary for studying quantum mechanics. We will first discuss Newtonian motion and cast this into the Lagrangian form. We will then discuss the principle of least action and Hamiltonian dynamics and the concept of phase space.

1.1 Newton's equations of motion

Newton's Principia set the theoretical basis of mathematical mechanics and analysis of physical bodies. The equation that force equals mass times acceleration is the fundamental equation of classical mechanics. Stated mathematically

$$\vec{F}(r) = m \frac{d^2 \vec{r}}{dt^2} = m \frac{d\vec{v}}{dt} = m\vec{a} \quad 1.1$$

where the force vector $\vec{F}(r)$ has components in all three dimensions and varies with location.

We can also define a position vector,

$$\vec{r} = \vec{x} + \vec{y} + \vec{z} \quad 1.2$$

and velocity vector

$$\vec{v} = \left(\frac{dx}{dt}\right) \hat{x} + \left(\frac{dy}{dt}\right) \hat{y} + \left(\frac{dz}{dt}\right) \hat{z} \text{ or } \vec{v} = \dot{x}\hat{x} + \dot{y}\hat{y} + \dot{z}\hat{z} \quad 1.3$$

For now we are limiting ourselves to one particle moving in one dimension. For motion in more dimensions, we need to introduce vector components. In cartesian coordinates, Newton's equations are

$$\begin{aligned} F_x &= m \frac{d^2 x}{dt^2} = m\ddot{x}, \\ F_y &= m \frac{d^2 y}{dt^2} = m\ddot{y}, \\ F_z &= m \frac{d^2 z}{dt^2} = m\ddot{z} \end{aligned} \quad 1.4$$

We can also replace the second-order differential equation with two first order equations.

$$\frac{d^2 x}{dt^2} = \frac{dv_x}{dt} = \dot{v}_x = \frac{F_x}{m} \quad 1.5$$

These, along with the initial conditions, $x(0)$ and $v(0)$ are all that are needed to solve for the motion of a particle with mass m given a force f . We could have chosen two end points as well and asked, what path the particle must take to get from one point to the next. Let us consider some elementary solutions.

1.1.1 Elementary solutions

First the case in which $F = 0$ and $\frac{d^2 x}{dt^2} = \ddot{x} = 0$. Thus,

$$\frac{dx}{dt} = \dot{x} = v_x = \text{constant} \quad 1.6$$

So, unless there is an applied force, the velocity of a particle will remain unchanged.

Second, we consider the case of a linear force, $F = -kx$. This is restoring force for a spring and such force laws are termed Hooke's law and k is termed the force constant. By substituting $F = -kx$ into eq. 1.4, then we have

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

$$\frac{d^2x}{dt^2} = -kx/m \tag{1.6}$$

So we want some function which is its own second derivative multiplied by a constant or a number. The cosine and sine functions have this property, so let's try

$$x(t) = A\cos(\omega t) + B\sin(\omega t) \tag{1.7}$$

Taking time derivatives

$$\frac{dx}{dt} = -\omega[-A\sin(\omega t) + B\cos(\omega t)] \tag{1.8}$$

$$\frac{d^2x}{dt^2} = -\omega^2[A\cos(\omega t) + B\sin(\omega t)] = -\omega^2x(t) \tag{1.9}$$

When comparing eq. 1.9 with eq. 1.6 and eq.1.8 with 1.3, we can easily obtain that

$$\omega = \sqrt{k/m} \tag{1.10}$$

and

$$v_x = \omega[-A\sin(\omega t) + B\cos(\omega t)] \tag{1.11}$$

Notice that the term $\sqrt{k/m}$ has units of angular frequency (s, second) ($\sqrt{(N/m)/kg}$
 $= \sqrt{(kg) \cdot (\frac{m}{s^2})/m}/kg = 1/s$).

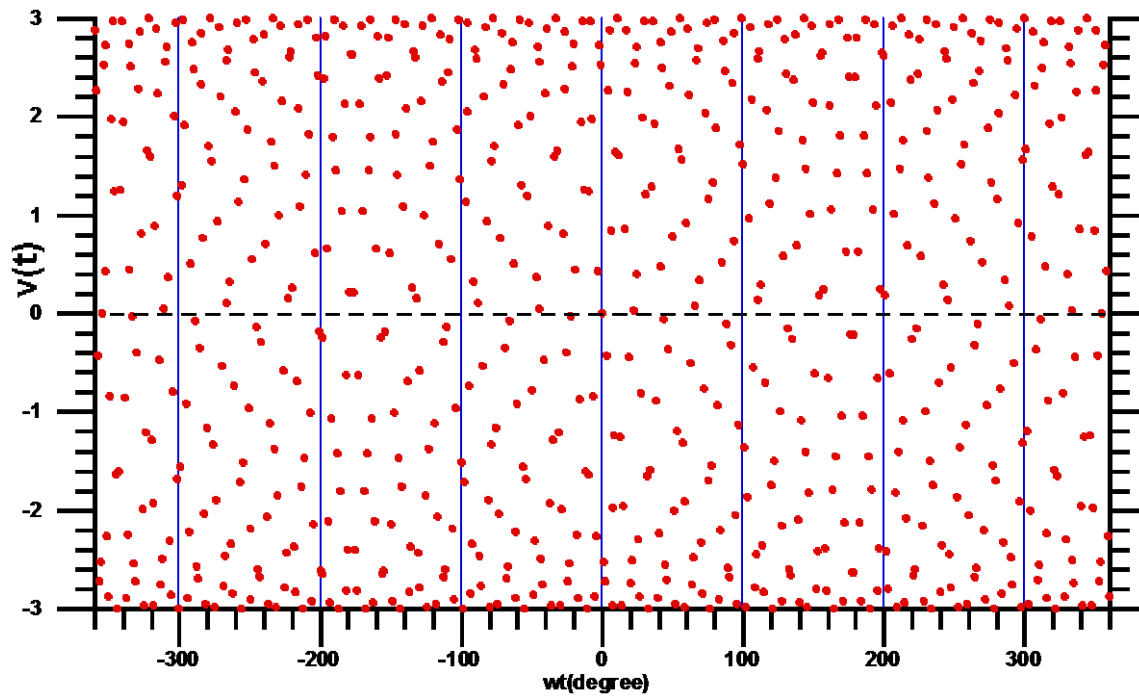
In order to determine coefficients A and B, we need two initial. Let's pick $x(0) = x_0$ and $v(0) = 0$. Thus,

$$x(t = 0) = x_0 = A\cos(\omega \cdot 0) + B\sin(\omega \cdot 0) = A \cdot 1 + B \cdot 0 = A$$

$$x(t) = x_0\cos(\omega t) \tag{1.12}$$

So, the equation of motion is

$$v_x(t) = -\omega x_0\sin(\omega t) \tag{1.13}$$



gauge

Tangent field for simple swing with $\omega = 1$. The superimposed curve is a linear approximation to the pendulum motion, $v_x(t) = -\omega x_0 \sin(\omega t)$

1.1.2 Phase plane analysis

Often one cannot determine the closed form solution to a given problem and we need to turn to more approximate methods or even graphical methods. Here, we will look at an extremely useful way to analyze a system of equations by plotting their time-derivatives.

First, let's look at the oscillator we just studied. We can define a vector s ,

$$s = (\dot{x}, \dot{v}) = \left(v, -\frac{k}{mx} \right) \quad 1.14$$

and plot the vector field as seen in the figure below. The superimposed curve is one trajectory and the arrows give the “flow” of trajectories on the phase plane.

We can examine more complex behavior using following procedure. For example, the simple pendulum obeys the equation

$$\frac{d^2x}{dt} = -\omega^2 \sin(x) \quad 1.15$$

This can be reduced to two first order equations:

$$\begin{aligned} \dot{x} &= v \\ \dot{v} &= -\omega^2 \sin(x) \end{aligned} \quad 1.16$$

We can approximate the motion of the pendulum for small displacements by expanding the pendulum's force about $x = 0$

$$\dot{v} = -\omega^2 \sin(x) = -\omega^2 \left(x - \frac{x^3}{6} + \dots \right)$$

For small x the cubic term is very small, and we have

$$\dot{v} = -\omega^2 \left(x - \frac{x^3}{6} + \dots \right) = -\omega^2 x = -\left(\frac{k}{m}\right)x \quad 1.17$$

which is the equation for harmonic motion. So, for small initial displacements, we see that the pendulum oscillates back and forth with an angular frequency ω . For large initial displacements, $x_0 = \pi$ or if we impart some initial velocity on the system $v_0 > 1$, the pendulum does not oscillate back and forth, but undergoes librational motion (spinning!) in one direction or the other.

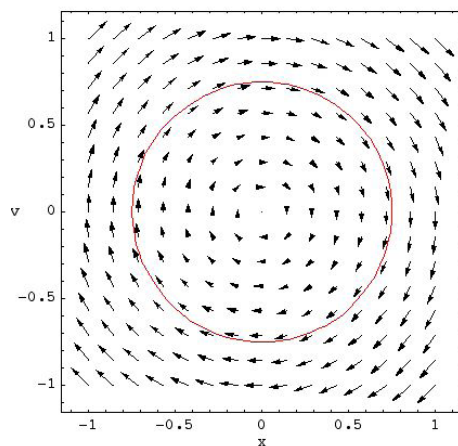
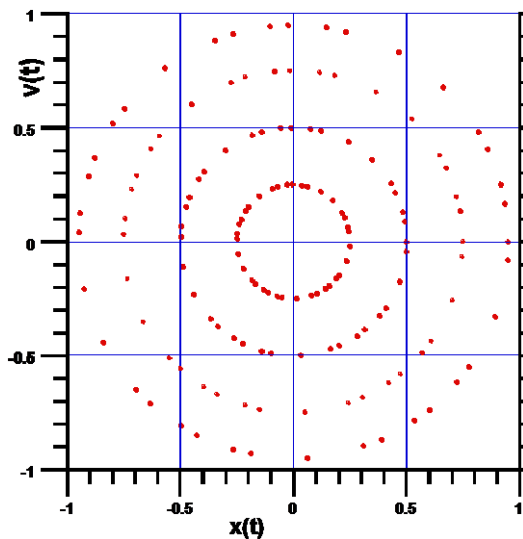


Figure: Screen shot of using Mathematica to plot phase-plane for harmonic oscillator. Here $k/m = 1$ and our $x_0 = 0.75$.

1.2 Lagrangian Mechanics

1.2.1 The Principle of Least Action

The most general form of the law governing the motion of a mass is the principle of least action or Hamilton's principle. The basic idea is that every mechanical system is described by a single function of coordinate, velocity, and time: $L(x, \dot{x}, t)$ and that the motion of the particle is such that certain conditions are satisfied. That condition is that the time integral of this function, takes the least possible value give a path that starts at x_0 at the initial time and ends at x_f at the final time.

$$S = \int_{t_0}^{t_f} L(x, \dot{x}, t) dt \quad 1.18$$

Lets take $x(t)$ be function for which S is minimized. This means that S must increase for any variation about this path, $x(t) + \delta x(t)$. Since the end points are specified, $\delta x(0) = \delta x(t) = 0$ and the change in S upon replacement of $x(t)$ with $x(t) + \delta x(t)$ is

$$\delta S = \int_{t_0}^{t_f} L(x + \delta x, \dot{x} + \delta \dot{x}, t) dt - \int_{t_0}^{t_f} L(x, \dot{x}, t) dt = 0 \quad 1.19$$

This is zero, because S is a minimum. Now, we can expand the integrand in the first term

$$L(x + \delta x, \dot{x} + \delta \dot{x}, t) = L(x, \dot{x}, t) + \left(\frac{\partial L}{\partial x} \delta x + \frac{\partial L}{\partial \dot{x}} \delta \dot{x} \right) \quad 1.20$$

Thus, we have

$$\int_{t_0}^{t_f} \left(\frac{\partial L}{\partial x} \delta x + \frac{\partial L}{\partial \dot{x}} \delta \dot{x} \right) dt = 0 \quad 1.21$$

Since $\delta \dot{x} = d\delta x/dt$ and integrating the second term by parts

$$\delta S = \left[\frac{\partial L}{\partial \dot{x}} \delta x \right]_{t_0}^{t_f} + \int_{t_0}^{t_f} \left(\frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} \right) \delta x dt = 0 \quad 1.22$$

The surface term vanishes because of the condition imposed above. This leaves the integral. It too must vanish and the only way for this to happen is if the integrand itself vanishes. Thus we have the

$$\frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} = 0 \quad 1.23$$

L is known as the Lagrangian. Before moving on, we consider the case of a free particle. The Lagrangian in this case must be independent of the position of the particle since a freely moving particle defines an inertial frame. Since space is isotropic, L must only depend upon the magnitude of v and not its direction. Hence, $L = L(v^2)$

Since L is independent of x , $\frac{\partial L}{\partial x} = 0$, so the Lagrange equation is

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{x}} = \frac{d}{dt} \frac{\partial L}{\partial v} = 0 \quad 1.24$$

So, $\frac{\partial L}{\partial v} = \text{constant}$ which leads us to conclude that L is quadratic in v . In fact,

$$L = \frac{1}{2} m v^2 \quad 1.25$$

which is the kinetic energy for a particle.

$$T = \frac{1}{2}mv^2 = \frac{1}{2}m\dot{x}^2 \quad 1.26$$

For a particle moving in a potential field, V , the Lagrangian is given by

$$L = T - V \quad 1.27$$

L has units of energy and gives the difference between the energy of motion and the energy of location.

This leads to the equations of motion:

$$\frac{d}{dt} \frac{\partial L}{\partial v} - \frac{\partial L}{\partial x} = \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} = 0 \quad 1.28$$

Substituting $L = T - V$, yields

$$m\ddot{x} = m\dot{v} = -\frac{\partial V}{\partial x} \quad 1.29$$

which is identical to Newton's equations given above once we identify the force as the minus the derivative of the potential. For the free particle, $\dot{x} = v = \text{constant}$. Thus,

$$S = \int_{t_0}^{t_f} \frac{1}{2}mv^2 dt = \frac{1}{2}mv^2(t_f - t_0) \text{ or}$$

$$S = \int_{t_0}^{t_f} \frac{1}{2}m\dot{x}^2 dt = \frac{1}{2}m\dot{x}^2(t_f - t_0) \quad 1.30$$

Reader may be wondering at this point why we needed a new function and derived all this from some minimization principle. The reason is that for some systems we have constraints on the type of motion they can undertake. For example, there may be bonds, hinges, and other mechanical difficulties which limit the range of motion a given particle can take. The Lagrangian formalism provides a mechanism for incorporating these extra effects in a consistent and correct way. In fact we will use this principle later in deriving a variational solution to the Schrodinger equation by constraining the wavefunction solutions to be orthonormal.

Lastly, it is interesting to note that $v^2 = \dot{\vec{r}}^2 = \left(\frac{d\vec{r}}{dt}\right)^2$ is the square of the element of an arc in a given coordinate system. Thus, within the Lagrangian formalism it is easy to convert from one coordinate system to another. For example, in cartesian coordinates:

$$(d\vec{r})^2 = dx^2 + dy^2 + dz^2 \quad 1.31$$

$$\text{Thus, } v^2 = \dot{\vec{r}}^2 = \dot{x}^2 + \dot{y}^2 + \dot{z}^2.$$

In cylindrical coordinates,

$$(d\vec{r})^2 = d\rho^2 + \rho d\phi^2 + dz^2 \quad 1.32$$

Then, we have the Lagrangian L

$$L = \frac{1}{2}m(d\vec{r})^2 = \frac{1}{2}m(\dot{\rho}^2 + \rho\dot{\phi}^2 + \dot{z}^2) \quad 1.33$$

For spherical coordinates

$$(d\vec{r})^2 = dr^2 + r^2 d\theta^2 + r^2 \sin^2 \theta d\phi^2 \quad 1.34$$

Therefore,

$$L = \frac{1}{2} m \left(\frac{d\vec{r}}{dt} \right)^2 = \frac{1}{2} m (\dot{r}^2 + r^2 \dot{\theta}^2 + (r^2 \sin^2 \theta) \dot{\phi}^2) \quad 1.35$$

1.2.2 Example: 3 dimensional harmonic oscillator in spherical coordinates

Here we take the potential energy to be a function of r alone (isotropic)

$$V(r) = \frac{1}{2} k r^2 \quad 1.36$$

Thus, the Lagrangian in cartesian coordinates is

$$L = T - V(r) = \frac{1}{2} m \dot{r}^2 - \frac{1}{2} k r^2 \quad 1.37$$

$$\vec{r}^2 = r^2 = x^2 + y^2 + z^2 \quad 1.38$$

$$\dot{\vec{r}}^2 = \dot{r}^2 = v^2 = \dot{x}^2 + \dot{y}^2 + \dot{z}^2. \quad 1.40$$

$$\begin{aligned} L &= \frac{1}{2} m \dot{r}^2 - \frac{1}{2} k r^2 \\ &= \left(\frac{1}{2} m \dot{x}^2 - \frac{1}{2} k x^2 \right) + \left(\frac{1}{2} m \dot{y}^2 - \frac{1}{2} k y^2 \right) + \left(\frac{1}{2} m \dot{z}^2 - \frac{1}{2} k z^2 \right) \end{aligned} \quad 1.41$$

If the system is separable into 3 independent oscillators, it can be converted to spherical polar coordinates such as:

So,

$$\begin{aligned} z &= r \cos \theta, \\ x &= (r \sin \theta) \cos \phi, \end{aligned} \quad 1.41$$

$$y = (r \sin \theta) \sin \phi,$$

and

$$\begin{aligned} \dot{z} &= \dot{r} \cos \theta - r \dot{\theta} \sin \theta, \\ \dot{x} &= \dot{r} \sin \theta \cos \phi - r \dot{\theta} \sin \theta \cos \phi - r \dot{\phi} \sin \theta \sin \phi \end{aligned} \quad 1.42$$

$$\dot{y} = \dot{r} \sin \theta \sin \phi + r \dot{\theta} \sin \theta \sin \phi + r \dot{\phi} \sin \theta \cos \phi,$$

$$L = \frac{1}{2} m (d\vec{r})^2 = \frac{1}{2} m (\dot{r}^2 + r^2 \dot{\theta}^2 + (r^2 \sin^2 \theta) \dot{\phi}^2) - \frac{1}{2} k r^2 \quad 1.43$$

The equations of motion are

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{r}} - \frac{\partial L}{\partial r} = \frac{d}{dt} (m \dot{r}) - m r \dot{\theta}^2 - m r \dot{\phi}^2 \sin^2 \theta + k r = 0 \quad 1.44$$

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{\theta}} - \frac{\partial L}{\partial \theta} = \frac{d}{dt} (m r^2 \dot{\theta}) - m r^2 \dot{\phi} \sin \theta \cos \theta + k r = 0 \quad 1.45$$

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{\phi}} - \frac{\partial L}{\partial \phi} = \frac{d}{dt} (m r^2 \dot{\phi} \sin^2 \theta) = 0 \quad 1.46$$

We now prove that the motion of a particle in a central force field lies in a plane containing the origin. The force acting on the particle at any given time is in a direction towards the origin. Now, place an arbitrary cartesian frame centered about the particle with the z axis parallel to the direction of motion as sketched in Fig. 1.2 Note that the y axis is perpendicular to the plane of the page and hence there is no force component in that direction.

Consequently, the motion of the particle is constrained to lie in the zx plane, i.e. the plane of the page and there is no force component which will take the particle out of this plane.

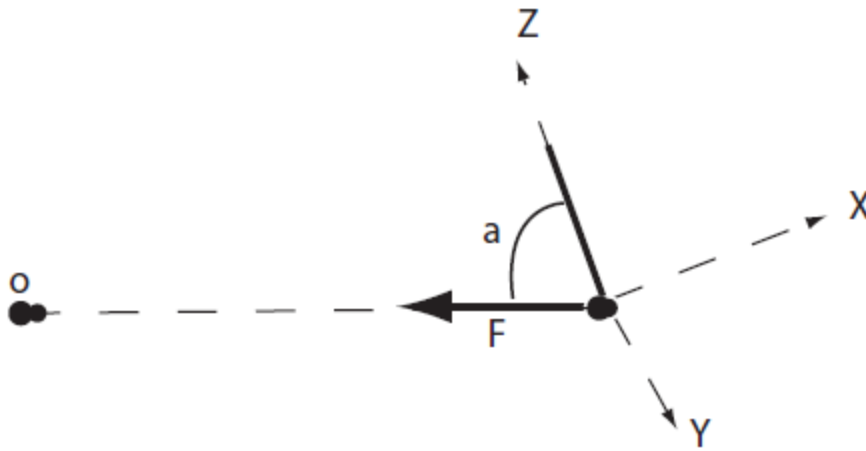


Figure 1.2: Vector diagram for motion in a central forces. The particle's motion is along the Z axis which lies in the plane of the page.

Let's make a change of coordinates by rotating the original frame to a new one whereby the new z' is perpendicular to the plane containing the initial position and velocity vectors. In the sketch above, this new z' axis would be perpendicular to the page and would contain the y axis we placed on the moving particle. In terms of these new coordinates, the Lagrangian will have the same form as before since our initial choice of axis was arbitrary. However, now, we have some additional constraints. Because the motion is now constrained to lie in the $x'y'$ plane, $\theta' = \pi/2$ is a constant, and $d\theta'/dt = 0$. Thus $\cos(\theta'/2) = 0$ and $\sin(\theta'/2) = 1$ in the equations above. From the equations for ϕ we find

$$\frac{d}{dt}(mr^2\dot{\phi})=0 \quad 1.47$$

$$mr^2\dot{\phi} = \text{constant} = P_{\phi}(\text{or } J) = \text{angular momentum}$$

This we can put the r into eq. 1.44 (here $\theta = \pi/2$), we get

$$\frac{d}{dt}(m\dot{r}) - mr\dot{\phi}^2 + kr = \frac{d}{dt}(m\dot{r}) - \frac{P_{\phi}^2}{mr^3} + kr = 0 \quad 1.48$$

where we notice that $-\frac{P_{\phi}^2}{mr^3}$ is the centrifugal force. Taking the last equation, multiplying by \dot{r} .

$$\dot{r} \frac{d}{dt}(m\dot{r}) - \dot{r} \frac{P_{\phi}^2}{mr^3} + kr\dot{r} = \dot{r} \frac{d}{dt}(m\dot{r}) - \frac{P_{\phi}^2}{mr^3} \left(\frac{dr}{dt}\right) + kr \left(\frac{dr}{dt}\right) = 0$$

$$\dot{r}d(m\dot{r}) - \frac{P_{\phi}^2}{mr^3}dr + krdr=0$$

or

$$\dot{r}d(m\dot{r}) - \frac{P_{\theta}^2}{mr^3}dr + krdr = 0$$

$$d\left(\frac{1}{2}m\dot{r}^2\right) - \frac{P_{\theta}^2}{mr^3}dr + krdr = 0 \quad 1.49$$

Integration of eq.1.49 gives, we have

$$\int d\left(\frac{1}{2}m\dot{r}^2\right) = \int \left(\frac{P_{\theta}^2}{mr^3} - kr\right) dr$$

$$\frac{1}{2}m\dot{r}^2 = -\frac{P_{\theta}^2}{2mr^2} - \frac{1}{2}kr^2 + b \quad \text{where } b \text{ is the constant of integration}$$

or

$$\dot{r}^2 = -\frac{P_{\theta}^2}{m^2r^2} - \frac{kr^2}{m} + b$$

$$\dot{r} = \sqrt{-\frac{P_{\theta}^2}{m^2r^2} - \frac{kr^2}{m} + b} \quad 1.50$$

Integrating eq.150 with respect to time,

$$\dot{r} = \frac{dr}{dt} = \sqrt{-\frac{P_{\theta}^2}{m^2r^2} - \frac{kr^2}{m} + b}$$

$$\int_{t_0}^t dt = \int \frac{dr}{\sqrt{-\frac{P_{\theta}^2}{m^2r^2} - \frac{kr^2}{m} + b}} = \frac{1}{2} \int \frac{dx}{\sqrt{a+bx+cx^2}}$$

$$t - t_0 = \frac{1}{2} \int \frac{dx}{\sqrt{a+bx+cx^2}} \quad 1.51$$

$$x = r^2, a = -\frac{P_{\theta}^2}{m^2} \text{ and } c = -k/m.$$

This is a standard integral and we can evaluate it to find

$$r^2 = \frac{1}{2\omega} [b + A \sin(\omega(t - t_0))]$$

$$\text{Where } A = \sqrt{b^2 - \frac{\omega^2 P_{\theta}^2}{m^2}}$$

What we see then is that r follows an elliptical path in a plane determined by the initial velocity.

This example also illustrates another important point which has tremendous impact on molecular quantum mechanics, namely, the angular momentum about the axis of rotation is conserved. We can choose any axis we want. In order to avoid confusion, let us define χ as the angular rotation about the body-fixed Z' axis and $_$ as angular rotation about the original Z axis. So our conservation equations are

$$mr^2\dot{\chi} = P_{\chi}$$

Out the Z' axis and

$$(mr^2 \sin \theta) \dot{\phi} = P_\phi$$

for some arbitrary fixed Z axis. The angle θ will also have an angular momentum associated with it $P_\theta = mr^2 \dot{\theta}$, but we do not have an associated conservation principle for this term since it varies with ϕ . We can connect P_χ with P_θ and P_ϕ about the other axis via

$$P_\chi d\chi = P_\theta d\theta + P_\phi d\phi$$

Consequently,

$$mr^2 \dot{\chi}^2 d\chi = mr^2 (\dot{\theta} d\theta + \dot{\phi} \sin \theta d\phi)$$

Here we see that the the angular momentum vector remains fixed in space in the absence of any external forces. Once an object starts spinning, its axis of rotation remains pointing in a given direction unless something acts upon it (torque), in essence in classical mechanics we can fully specify $L_x, L_y,$ and L_z as constants of the motion since $\frac{d\vec{L}}{dt} = 0$. In a later chapter, we will cover the quantum mechanics of rotations in much more detail. In the quantum case, we will find that one cannot make such a precise specification of the angular momentum vector for systems with low angular momentum. We will, however, recover the classical limit in end as we consider the limit of large angular momenta.

1.3 Conservation Laws

We just encountered one extremely important concept in mechanics, namely, that some quantities are conserved if there is an underlying symmetry. Next, we consider a conservation law arising from the homogeneity of time. For a closed dynamical system, the Lagrangian does not explicitly depend upon time. Thus we can write

$$\frac{dL}{dt} = \frac{\partial L}{\partial x} \dot{x} + \frac{\partial L}{\partial \dot{x}} \ddot{x}$$

Replacing $\frac{\partial L}{\partial x}$ with Lagrange's equation, we obtain

$$\frac{dL}{dt} = \dot{x} \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}} \right) + \frac{\partial L}{\partial \dot{x}} \ddot{x} = \frac{d}{dt} \left(\dot{x} \frac{\partial L}{\partial \dot{x}} \right)$$

Now, rearranging this a bit,

$$\frac{d}{dt} \left(\dot{x} \frac{\partial L}{\partial \dot{x}} - L \right) = 0$$

So, we can take the quantity in the parenthesis to be a constant.

$$E = \left(\dot{x} \frac{\partial L}{\partial \dot{x}} - L \right) = \text{constant}$$

is an integral of the motion. This is the energy of the system. Since L can be written in form

$L = T - V$ where T is a quadratic function of the velocities, and using Euler's theorem on homogeneous functions:

$$\dot{x} \frac{\partial L}{\partial \dot{x}} = \dot{x} \frac{\partial(T-V)}{\partial \dot{x}} = \dot{x} \frac{\partial T}{\partial \dot{x}} = 2T$$

Thus,

$$E = \left(\dot{x} \frac{\partial L}{\partial \dot{x}} - L \right) = 2T - (T - V) = T + V = \text{constant}$$

which says that the energy of the system can be written as the sum of two different terms: the kinetic energy or energy of motion and the potential energy or the energy of location.

One can also prove that linear momentum is conserved when space is homogeneous. That is, when we can translate our system some arbitrary amount ε and our dynamical quantities must remain unchanged. We will prove this in the problem sets.

1.4 Hamiltonian Dynamics

Hamiltonian dynamics is a further generalization of classical dynamics and provides a crucial link with quantum mechanics. Hamilton's function, H , is written in terms of the particle's position and momentum, $H = H(p, q)$. It is related to the Lagrangian via

$$H = \dot{x}P - L(x, \dot{x})$$

Taking the derivative of H with respect to x (NOTE that $F_x = m\ddot{x} = \frac{d(m\dot{x})}{dt} = \dot{p} =$

$$-\frac{dV}{dx} \text{ and } q = x)$$

$$\frac{\partial H}{\partial x} = -\frac{\partial L}{\partial x} = -\dot{p}$$

Differentiation with respect to p gives

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

These last two equations give the conservation conditions in the Hamiltonian formalism. If H is independent of the position of the particle, then the generalized momentum, p is constant in time. If the potential energy is independent of time, the Hamiltonian gives the total energy of the system,

$$H = T + V$$

1.4.1 Interaction between a charged particle and an electromagnetic field.

We consider here a free particle with mass m and charge e in an electromagnetic field. The Hamiltonian is

$$H = \dot{x}P_x + \dot{y}P_y + \dot{z}P_z - L = \dot{x} \frac{\partial L}{\partial \dot{x}} + \dot{y} \frac{\partial L}{\partial \dot{y}} + \dot{z} \frac{\partial L}{\partial \dot{z}} - L$$

Our goal is to write this Hamiltonian in terms of momenta and coordinates.

For a charged particle in a field, the force acting on the particle is the Lorenz force. Here it is useful to introduce a vector and scalar potential and to work in cgs units.

$$\vec{F} = \frac{e}{c} \vec{v} \times (\vec{\nabla} \times \vec{A}) - \frac{e}{c} \frac{\partial \vec{A}}{\partial t} - e \vec{\nabla} \phi$$

The force in the x direction is given by

$$F_x = \frac{d(m\dot{x})}{dt} = \frac{e}{c} \left(\dot{y} \frac{\partial A_y}{\partial x} + \dot{z} \frac{\partial A_z}{\partial x} \right) - \frac{e}{c} \left(\dot{y} \frac{\partial A_x}{\partial y} + \dot{z} \frac{\partial A_x}{\partial z} + \frac{\partial A_x}{\partial t} \right) - e \frac{\partial \phi}{\partial x}$$

with the remaining components given by cyclic permutation. Note: $\vec{a} \times (\vec{b} \times \vec{c}) = \vec{b}(\vec{a} \cdot \vec{c}) - (\vec{a} \cdot \vec{b})\vec{c}$

Since

$$\frac{dA_x}{dt} = \frac{\partial A_x}{\partial t} + \dot{x} \frac{\partial A_x}{\partial x} + \dot{y} \frac{\partial A_x}{\partial y} + \dot{z} \frac{\partial A_x}{\partial z}$$

$$F_x = \frac{e}{c} \left(\dot{x} \frac{\partial A_x}{\partial x} + \dot{y} \frac{\partial A_x}{\partial y} + \dot{z} \frac{\partial A_x}{\partial z} \right) - \frac{e}{c} \vec{v} \cdot \vec{A} - e \frac{\partial \phi}{\partial x}$$

$$\vec{F} = \left\{ \frac{e}{c} \frac{d\vec{A}}{dt} - \frac{e}{c} \vec{\nabla}(\vec{v} \cdot \vec{A}) - e \vec{\nabla} \phi \right\}$$

Based upon this, we find that the Lagrangian is

$$L = \frac{1}{2} m \dot{x}^2 + \frac{1}{2} m \dot{y}^2 + \frac{1}{2} m \dot{z}^2 + \frac{e}{c} \vec{v} \cdot \vec{A} - e \phi$$

where ϕ is a velocity independent and static potential.

Continuing on, the Hamiltonian is

$$H = \frac{1}{2} m \dot{x}^2 + \frac{1}{2} m \dot{y}^2 + \frac{1}{2} m \dot{z}^2 + e \phi = \frac{1}{2m} [(m\dot{x})^2 + (m\dot{y})^2 + (m\dot{z})^2] + e \phi$$

The velocities, $m\dot{x}$, are derived from the Lagrangian via the canonical relation

$$P_x = \frac{\partial L}{\partial \dot{x}}$$

From this we find,

$$m\dot{x} = P_x - \frac{e}{c} A_x$$

$$m\dot{y} = P_y - \frac{e}{c} A_y$$

$$m\dot{z} = P_z - \frac{e}{c} A_z$$

and the resulting Hamiltonian is:

$$H = \frac{1}{2m} \left[\left(P_x - \frac{e}{c} A_x \right)^2 + \left(P_y - \frac{e}{c} A_y \right)^2 + \left(P_z - \frac{e}{c} A_z \right)^2 \right] + e \phi$$

$$\text{or } m\dot{\vec{r}} = \vec{P} - \frac{e}{c} \vec{A}$$

$$H = \frac{1}{2m} \left| \vec{P} - \frac{e}{c} \vec{A} \right|^2 + e \phi$$

We see here an important concept relating the velocity and the momentum. In the absence of a vector potential, the velocity and the momentum are parallel. However, when a vector

potential is included, the actual velocity of a particle is no longer parallel to its momentum and is in fact deflected by the vector potential.

Appendix	
2 Lorentz Force Law	
The Lorentz force in Gaussian Units is given by:	
$\vec{F} = -e(\vec{E} + \frac{\vec{v}}{c} \times \vec{B})$	a1
where Q is the electric charge, $\vec{E}(x, t)$ is the electric field and $\vec{B}(x, t)$ is the magnetic field. If the sources (charges or currents) are far away, $\vec{E}(x, t)$ and $\vec{B}(x, t)$ solve the homogeneous Maxwell equations. In Gaussian Units, they are given by	
$\vec{\nabla} \cdot \vec{B} = 0$	a2
$\vec{\nabla} \times \vec{E} + \frac{1}{c} \frac{\partial \vec{B}}{\partial t} = 0$	a3
The magnetic field \vec{B} can be derived from a <i>vector potential</i> \vec{A} :	
$\vec{B} = \vec{\nabla} \times \vec{A}$	a4
If we plug this into Eq. (a3), we get	
$\vec{\nabla} \times \left(\vec{E} + \frac{1}{c} \frac{\partial \vec{A}}{\partial t} \right) = 0$	a5
So the expression in square brackets is a vector field with no curl and can be written as the gradient of a <i>scalar potential</i> ϕ :	
$\vec{E} + \frac{1}{c} \frac{\partial \vec{A}}{\partial t} = -\vec{\nabla} \phi$	a6
or	
$\vec{E} = -\frac{1}{c} \frac{\partial \vec{A}}{\partial t} - \vec{\nabla} \phi$	a7
This we plug into Eq. (a1) for the Lorentz force law and we get	
$\vec{F} = e \left\{ \frac{1}{c} \left[\frac{\partial \vec{A}}{\partial t} - \vec{v} \times (\vec{\nabla} \times \vec{A}) \right] + \vec{\nabla} \phi \right\}$	a8
If we apply the general general vector relation	
$\vec{a} \times (\vec{b} \times \vec{c}) = \vec{b}(\vec{a} \cdot \vec{c}) - (\vec{a} \cdot \vec{b})\vec{c}$	a9
to the triple vector cross product in the square brackets, we get	

$$\vec{v} \times (\vec{\nabla} \times \vec{A}) = \vec{\nabla}(\vec{v} \cdot \vec{A}) - (\vec{v} \cdot \vec{\nabla})\vec{A} \quad \text{a10}$$

So the equation for the Lorentz force law is now

$$\vec{F} = e \left\{ \frac{1}{c} \left[\frac{\partial \vec{A}}{\partial t} + (\vec{v} \cdot \vec{\nabla})\vec{A} - \vec{\nabla}(\vec{v} \cdot \vec{A}) \right] + \vec{\nabla}\phi \right\} \quad \text{a11}$$

Now let's look at the total time derivative of $\vec{A}(\vec{x}, t)$

$$\frac{d\vec{A}(\vec{x}, t)}{dt} = \frac{\partial \vec{A}(\vec{x}, t)}{\partial t} + \sum_i v_i \frac{\partial \vec{A}(\vec{x}, t)}{\partial x_i} \quad \text{where } \sum_i v_i \frac{\partial \vec{A}(\vec{x}, t)}{\partial x_i} = (\vec{v} \cdot \vec{\nabla})\vec{A}(\vec{x}, t) \quad \text{a12}$$

$$\frac{d\vec{A}(\vec{x}, t)}{dt} = \frac{\partial \vec{A}(\vec{x}, t)}{\partial t} + (\vec{v} \cdot \vec{\nabla})\vec{A}(\vec{x}, t) \quad \text{a13}$$

The right side of the equation corresponds to the first two terms in the square brackets of Eq. (a11), and we can write

$$\vec{F} = e \left\{ \frac{1}{c} \frac{d\vec{A}}{dt} + \frac{1}{c} \vec{\nabla}(\vec{v} \cdot \vec{A}) + \vec{\nabla}\phi \right\} \quad \text{a14}$$

1.4.3 Virial Theorem

Finally, we turn our attention to a concept which has played an important role in both quantum and classical mechanics. Consider a function G that is a product of linear momentum and coordinate,

$$G = pq$$

The time derivative is simply,

$$\frac{dG}{dt} = \dot{G} = \dot{p}q + p\dot{q}$$

Now, let's take a time average of both sides of this last equation.

$$\langle \dot{G} \rangle = \left\langle \frac{d}{dt}(pq) \right\rangle = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \frac{d}{dt}(pq) dt = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T d(pq)$$

$$\langle \dot{G} \rangle = \left\langle \frac{d}{dt}(pq) \right\rangle = \lim_{T \rightarrow \infty} \frac{1}{T} [(pq)_T - (pq)_0]$$

If the trajectories of system are bounded, both p and q are periodic in time and are therefore finite. Thus, the average must vanish as $T \rightarrow \infty$ giving

$$\langle \dot{p}q + p\dot{q} \rangle = 0$$

Since $p\dot{q} = 2T$ and $\dot{p} = -F$, then, we have

$$\langle 2T \rangle = -\langle qF \rangle$$

In cartesian coordinates, this leads to

$$\langle 2T \rangle = -\langle qF \rangle = -\langle \sum_i x_i F_i \rangle$$

For a conservative system, owing to $\vec{F} = -\vec{\nabla}V$, if we have a centro-symmetric potential given by $V = Cr^n$, it is easy to show that

$$\langle 2T \rangle = n \langle V \rangle$$

For the case of the Harmonic oscillator, $n = 2$ and $\langle T \rangle = \langle V \rangle$. So, for example, if we have a total energy equal to kT in this mode, then $\langle T \rangle + \langle V \rangle = kT$ and $\langle T \rangle = \langle V \rangle = kT/2$. Moreover, for the interaction between two opposite charges separated by r , $n = -1$ and $\langle 2T \rangle = -\langle V \rangle$.

Chapter 2

2 Waves and Wavefunctions

2.1. Waves on a String: Physical Motivation

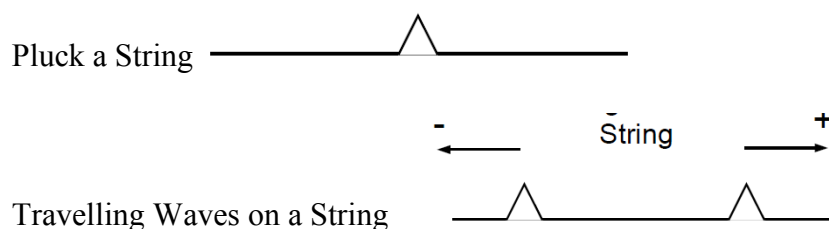
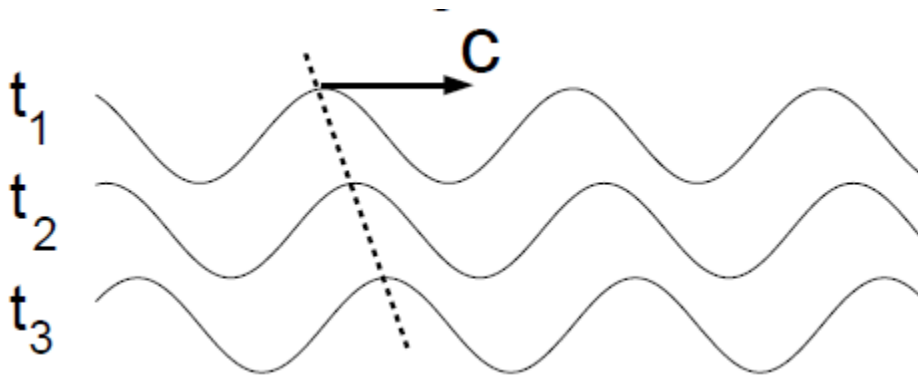


Figure 1: Two traveling waves are set in motion in opposite directions by plucking a string.

Let's begin with a brief review of what we all saw in basic physics as undergrads. Consider waves on a string. When you pluck a string, you send traveling waves in both directions as Figure 1 shows. If the string is finite and clamped at both ends, the traveling waves reflect at the clamping points and superpose to produce standing waves.

2.2 Travelling Sine-Waves



$$\phi(x, t) = \sin[kx - \omega t] = \sin[k(x - ct)] \text{ and } c = \omega/k$$

Figure 2: Illustration of a traveling sine-wave. The crest of the wave occurs where the phase is zero, which moves to the right with speed, $c = \frac{\omega}{k}$.

Similar to the traveling waves shown in Figure 1, sine-waves can also travel as Figure 2 shows. In fact, if we let $\phi(x; t)$ denote the displacement of the string in the vertical direction as a function of position along the string (x) and time (t), it's easy to see that the following expression is a traveling wave

$$\phi(x; t) = \sin(kx - \omega t) = \sin\left[k\left(x - \frac{\omega}{k}t\right)\right] = \sin[k(x - ct)] \quad 2.1$$

in which each wave-crest or trough moves with speed $c = \frac{\omega}{k}$ to the right. Here ω is angular frequency ($\omega = 2\pi\nu$) and k is wavenumber ($k = \frac{2\pi}{\lambda}$), where f is frequency in Hz and λ is wavelength, presumably in meters. To say that a sine-wave moves means that the peaks and troughs move, that is that the locations of constant phase move. The wave given by equation (1), therefore, is seen to move in the $+x$ direction, because the phase $k(x-ct)$ is constant only if x increases as t increases. In fact, it is constant only if x increases with speed c . Of course, similar expressions could be derived for a traveling cosine-wave: $\cos[k(x - ct)]$; $\cos[k(x + ct)]$.

We noted above that traveling waves on a clamped string superpose to produce a standing wave. If the traveling waves are sine-waves this is easy to show using a simple trig

identity ($\sin(a+b)=\sin a \cdot \cos b + \cos a \cdot \sin b$). Consider the superposition of two traveling sine-waves and apply the trig identity:

$$\begin{aligned} & \sin(kx - \omega t) + \sin(kx + \omega t) \\ &= [\sin kx \cos(-\omega t) + \cos kx \sin(-\omega t)] + [\sin kx \cos(\omega t) + \cos kx \sin(\omega t)] \\ &= [\sin kx \cos(\omega t) - \cos kx \sin(\omega t)] + [\sin kx \cos(\omega t) + \cos kx \sin(\omega t)] \\ &= 2\sin kx \cos \omega t; \end{aligned} \tag{2.2}$$

where we have also used the fact that cosine is a symmetric (or even) function around the origin and sine is anti-symmetric (or odd) so $\cos(-\omega t) = \cos(\omega t)$ and $\sin(-\omega t) = -\sin(\omega t)$. It should be apparent that $\sin kx \cdot \sin \omega t$ is also a standing wave, but is shifted $\pi/2$ (half a period) in time.

As equation (1) is the classical form for a traveling sine-wave, equation (2) is the form of a standing sine-wave. Note that there is no standing cosine ($\cos kx \cdot \sin \omega t$; $\cos kx \cdot \cos \omega t$) for a clamped string, because the cosine does not satisfy the boundary conditions that displacement goes to zero at the ends of the string. If the string would be unclamped at one end, then the standing cosine would be allowed.

From equation (2), we see that standing waves on a string are the product of a spatial shape ($\sin kx$) and a temporal harmonic or oscillation ($\cos \omega t$; $\sin \omega t$). The shape is sometimes called the eigenfunction. To this point, we've merely posited the shape being a sine and ruled out a cosine by consideration of the boundary conditions, but later in the notes we will derive the shape of the string. The shapes of several sines are shown in Figure 3. Each of these potential shapes of oscillation is called a normal mode or a mode of oscillation and can be denoted by a single number n , sometimes called the quantum number of the normal mode because the allowed shapes are discrete. The quantum numbers are integers $n = 1; 2; 3; \dots$ where $n = 1$ is the fundamental mode and $n \geq 2$ are the higher modes of oscillation. Inspection of Figure 3 shows that the wavelength of the fundamental mode is $\lambda_1 = 2a$ and the first higher modes are $\lambda_2 = a$; $\lambda_3 = 2a/3$, etc., and in general satisfy the following criterion:

$$\lambda_n = \frac{2a}{n}$$

from which the following can be deduced:

$$k_n = \frac{2\pi}{\lambda_n} = \frac{n\pi}{a} \text{ and } \omega_n = ck_n = \frac{n\pi c}{a} \tag{2.3}$$

Because the boundary conditions determine the wavelengths, they also determine the frequencies. This fact is commonly summarized by reporting that the boundary conditions are what determine the frequencies of oscillation, or eigenfrequencies.

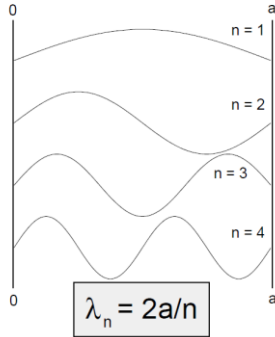


Figure 3: Modes of oscillation of a string clamped at both ends. Each mode has a shape of $\sin(n\pi x/a)$ with wavelength $2a/n$, where n is the modal index or quantum number that specifies the mode.

Note that we have shown that if each standing wave or normal mode on a string, $\phi_n(x; t)$, is the sum of two traveling waves then it is simply the product of a spatial shape and a temporal oscillation. Let's represent the spatial shape and temporal oscillation as $\phi_n(x)$ and $T_n(t)$ so that:

$$\phi_n(x; t) = \phi_n(x)T_n(t) = \sin k_n x (A_n \cos \omega_n t + B_n \sin \omega_n t) \quad 2.4$$

This is actually a rather powerful result, and doesn't hold for all phenomena, and in fact only holds for the string under certain restrictive conditions that we have implicitly assumed here (e.g., the equilibrium tension in the string does not change with time). This result, equation (4), is called the separation of variables and we'll use it later in solving the string equation more formally.

The actual displacement that the string would undergo if plucked or kicked would be a sum or superposition of the modes of oscillation as follows:

$$\begin{aligned} \phi_n(x; t) &= \sum_{n=1}^{\infty} \phi_n(x, t) = \sum_{n=1}^{\infty} \phi_n(x)T_n(t) \\ &= \sum_{n=1}^{\infty} \sin k_n x (A_n \cos \omega_n t + B_n \sin \omega_n t) \\ &= \sum_{n=1}^{\infty} \sin \left(\frac{n\pi x}{a} \right) \left(A_n \cos \left(\frac{n\pi c t}{a} \right) + B_n \sin \left(\frac{n\pi c t}{a} \right) \right) \end{aligned} \quad 2.5$$

Each coefficient A_n and B_n is a weight that determines both the relative contribution of each mode of oscillation to the final displacement and the phase of the temporal oscillation. These coefficients depend on how the string is set into motion; if it is plucked or kicked, for example. If, for example, you pluck a string near the node of a mode of oscillation, you will not excite that mode.

It is important to know that the way in which the string is set into motion is called the initial conditions and the initial conditions are what determine the A_n and B_n . Finding the A_n and B_n is easy if you know about Fourier Series, although it can be rather tedious. The initial shape of the string can be seen from equation (5) to be just the displacement at $t=0$,

$$\phi_n(x; t = 0) = \sum_{n=1}^{\infty} \sin\left(\frac{n\pi x}{a}\right)$$

This is simply the Fourier Series expansion of the initial displacement pattern of the string. So, if you can find the Fourier Series expansion of the initial displacement pattern, you have the A_n . Similarly, you can find the B_n from the initial velocity applied to the string, except you will need to take the Fourier Series expansion of the initial velocity pattern of the string, which is the time derivative of equation (5).

2.3 A Differential Equation (We've Seen Before)

The wave equation for a string is a differential equation. An example that you've seen before is the simple harmonic oscillator (Figure 4).

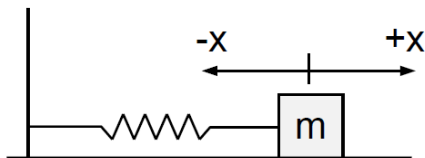


Figure 4: Schematic representation of a simple harmonic oscillator (SHO), in which a mass m , connected to a spring with spring-constant k , oscillates with displacement $\pm x$ about equilibrium.

For small displacements its motion can be modeled with Hooke's Law that says that the force is in the direction opposite to the displacement from equilibrium and has a magnitude proportional to the displacement ($F = -kx$). When this is placed into Newton's second law ($F = ma$) you get a differential equation as shown here:

$$m \frac{d^2 X(t)}{dt^2} = ma = F = -kX(t)$$

$$\frac{d^2X(t)}{dt^2} = -\frac{k}{a}X(t) = -\omega^2X(t) \quad 2.6$$

Equation (6) is sometimes called the simple harmonic oscillator (SHO) equation. The SHO, as we recall, oscillates with frequency $\omega = \sqrt{k/m}$. In the parlance of differential equations, it is a linear, second-order, homogeneous, ordinary differential equation with constant coefficients.

It is

- a differential equation because there are derivatives in it,
- ordinary because there are no partial derivatives in it (more on this later),
- second-order because its highest derivative with respect to the independent variable t is of second-order, homogeneous because the right-hand-side of the equation is zero which means physically
- homogeneous because the right-hand-side of the equation is zero which means physically that there are no applied forces, and, finally
- It has constant coefficients because the terms that multiply the functions of x are constant in this case it's $\omega^2 = k/m$.

Because this is a linear ODE, if $x_1(t)$ and $x_2(t)$ are solutions, so is $ax_1(t)+bx_2(t)$ where a ; b are arbitrary constants. Because it is a second-order ODE, there are two and only two independent solutions. Also within the parlance of differential equations, equations like equation (6) are called Helmholtz equations. Ordinary differential equations are often called ODEs. Helmholtz equations, like the SHO-equation, are particularly easy to solve. The trial solution can be written in a variety of equivalent ways, one of which is:

$$X(t) = A\cos\omega t + B_n \sin\omega t \quad 2.7$$

where $\omega^2 = \frac{k}{m}$ and A and B are arbitrary constants that depend on the initial conditions that is on how the oscillator has been set into motion (drag and let go or a kick, for example). Note that there are two independent solutions ($\cos\omega t$, $\sin\omega t$) whose linear combination is also a solution. We can show that equation (7) is a solution to equation (6) by direct substitution:

$$\frac{dX(t)}{dt} = -A\omega\sin\omega t + B\omega\cos\omega t$$

$$\frac{d^2X(t)}{dt^2} = \frac{d}{dt} \left(\frac{dX(t)}{dt} \right) = -\omega^2 (A \cos \omega t + B \sin \omega t) \quad 2.8$$

Substitution of equations (7) and (8) into (6) establishes the result:

$$\frac{d^2X(t)}{dt^2} + \omega^2 X(t) = -\omega^2 (A \cos \omega t + B \sin \omega t) + \omega^2 (A \cos \omega t + B \sin \omega t) = 0$$

The procedure that we followed here is actually similar to how differential equations are solved in practice, you guess a solution and see if it works. The guessed solution is often called the trial solution or *ansatz*, which is the fancier German name for it and you can use this to impress your friends who don't know any better. Now that we know the solution to Helmholtz equations like the SHO equation, we have a starting point for trial solutions later on.

2.4. Derivation of the 1-D Wave Equation for a String

Consider the displacement applied to a string of length L in a coordinate system shown in Figure 5. The displacement y is a function of time t and the spatial coordinate x : $\phi(x; t)$. Let ρ be the mass density of the string with units of mass per unit length and assume that ρ is constant. Let T be the tension in the string. Tension is a force and assume that when the string is plucked the tension remains constant throughout the string. This is the same as assuming that the displacement is small for a homogeneous string. Also, assume that the force of gravity is much weaker than tension ($\rho L g \ll T$) so that it does not affect the motion of the string appreciably and can, therefore, be ignored. Inspection of Figure 6 shows that the x - and y -components of force (i.e., tension) can be written as follows:

$$\text{x-tension } \sum F_x = T \cos \theta_2 - T \cos \theta_1 \quad 2.9$$

$$\text{y-tension } \sum F_y = T \sin \theta_2 - T \sin \theta_1 \quad 2.10$$



Figure 5: Coordinate system for a string of length L that will undergo vertical (or transverse) displacements $y(x; t)$.

We're interested in modeling the vertical motion of the string, $y(x; t)$, so we will explore the use of equation (10).

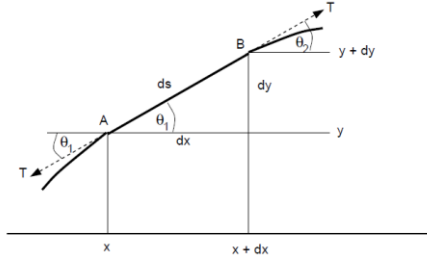


Figure 6:

Because the oscillations are small, the angles θ_1 and θ_2 are small. Thus, $\sin\theta_1 \approx \tan\theta_1$ and $\sin\theta_2 \approx \tan\theta_2$. We note that the increment of mass in length ds is just $m = \rho ds$. Again, because the oscillations are small, $ds \approx dx$ so $m \approx \rho dx$. We can, therefore, rewrite equation (10) as Newton's second law governing motion of the string in the y -direction:

$$ma_y = \rho dx \frac{\partial^2 y}{\partial x^2} = \sum F_y = T(\tan\theta_2 - \tan\theta_1) \quad 2.11$$

Inspection of Figure 6 again reveals that $\tan\theta \approx \frac{\partial y}{\partial x}$, thus we can rewrite equation (11) as:

$$\rho dx \frac{\partial^2 y}{\partial x^2} = T \left[\left(\frac{\partial y}{\partial x} \right)_B - \left(\frac{\partial y}{\partial x} \right)_A \right] \quad 2.12$$

Note that the slope of the string at point B can be expressed as a truncated Taylor Series expansion about point A:

$$\left(\frac{\partial y}{\partial x} \right)_B \approx \left(\frac{\partial^2 y}{\partial x^2} \right)_A dx + \left(\frac{\partial y}{\partial x} \right)_A \quad 2.13$$

Therefore,

$$\left(\frac{\partial^2 y}{\partial x^2} \right)_A dx = \left(\frac{\partial y}{\partial x} \right)_B - \left(\frac{\partial y}{\partial x} \right)_A \quad 2.14$$

Substituting equation (14) into equation (12), therefore, reveals that:

$$\rho \frac{\partial^2 y}{\partial t^2} = T \frac{\partial^2 y}{\partial x^2} \quad 2.15$$

where we cancelled the factor of dx on both sides of the equation. This equation holds at any location A along the string, so we have removed the subscript A and make location implicit in the function $y(x; t)$.

Both sides of equation (15) have units of force per unit length. If there are forces $F(t)$ applied to the string, they will be added to the right-hand-side of this equation, as follows:

$$\rho \frac{\partial^2 y}{\partial t^2} = T \frac{\partial^2 y}{\partial x^2} + F(t) \quad 2.16$$

where $F(t)$ has units of force per unit length.

Remember that the LHS is analogous to ma in Newton's second law so that the RHS represents the forces on the string. The first term on the RHS is the restoring force exerted on the displacement by the string itself. In the absence of applied forces (after the initial conditions), we get the equation for the free oscillations of a homogeneous string which can be rewritten as:

$$\frac{\partial^2 y}{\partial x^2} = \frac{\rho}{T} \frac{\partial^2 y}{\partial t^2} \quad \text{and} \quad \frac{\rho}{T} = \frac{1}{c^2} \quad \text{then, we have}$$

$$\frac{\partial^2 y}{\partial x^2} = \frac{1}{c^2} \frac{\partial^2 y}{\partial t^2} \quad 2.17$$

where $c = \sqrt{\frac{\rho}{T}}$ is the speed of propagation of the wave traveling in the $\pm x$ -direction.

Equation (17) is generally referred to as the 1-D wave equation. It says that the curvature of the string at spatio-temporal point $(x; t)$ is proportional to the vertical acceleration of the string at that point and that the constant of proportionality is related to the horizontal speed of propagation of a wave on the string. I don't know about you, but I wouldn't have guessed that.

All of this holds if the string is homogeneous, that is if the density and tension and, hence, the speed of a wave on the string are constant. If T and ρ are a function of position along the string, then the wave equation is

$$\rho(x) \frac{\partial^2 y}{\partial t^2} = \frac{\partial}{\partial x} \left(T(x) \frac{\partial y}{\partial x} \right) \quad 2.18$$

We will consider different methods to treat this case later on.

Here we have considered transverse oscillations. For longitudinal oscillations, $u(x)$, the result will be the same but the derivation will differ. For longitudinal waves, replace tension $T(x)$

with Young's modulus $k(x)$, which is analogous to the spring constant for the simple harmonic oscillator. For the longitudinal oscillations of an inhomogeneous string, therefore:

$$\rho(x) \frac{\partial^2 y}{\partial t^2} = \frac{\partial}{\partial x} \left(k(x) \frac{\partial y}{\partial x} \right) \quad 2.19$$

In this derivation, stress is assumed proportional to strain (Hooke's Law) and the constant of proportionality is k .

2.5. Solving the 1D Homogeneous Wave Equation with Separation of Variables

We now want to solve the wave equation in 1 spatial dimension (1-D), equation (17). This equation governs wave propagation in a 1-D medium, such as a string or a wire.

Partial differential equations such as equation (17) are usually not solved directly, but are transformed into other equations that can be solved. Usually they are transformed first into a set of ODEs, one for each free variable. For the 1-D wave equation, therefore, we'll expect two equations, one in x and one in t . The method we're going to follow now is called the method of separation of variables.

Equation (17) can be separated into these two constitutive equations by using the method of separation of variables in the following way. Let us assume that the solution can be written (as we know it can for a string) in terms of the product of two functions, one in x and the other in t , in the following way:

$$y(x; t) = Y(x)T(t) \quad 2.20$$

$Y(x)$ and $T(t)$ are the unknowns we wish to find and equation (20) is a kind of trial solution and we'll see if it works. To substitute equation (20) into equation (17) we'll first need the space and time derivatives of y :

$$\begin{aligned} \frac{\partial y(x,t)}{\partial x} &= T(t) \left(\frac{\partial Y(x)}{\partial x} \right) = T(t) \frac{dY(x)}{dx} \\ \frac{\partial^2}{\partial x^2} y(x, t) &= T(t) \left(\frac{\partial^2 Y(x)}{\partial x^2} \right) = T(t) \frac{d^2 Y(x)}{dx^2} \end{aligned} \quad 2.21$$

$$\begin{aligned} \frac{\partial y(x,t)}{\partial t} &= Y(x) \left(\frac{\partial T(t)}{\partial t} \right) = Y(x) \frac{dT(t)}{dt} \\ \frac{\partial^2}{\partial t^2} y(x, t) &= Y(x) \left(\frac{\partial^2 T(t)}{\partial t^2} \right) = Y(x) \frac{d^2 T(t)}{dt^2} \end{aligned} \quad 2.22$$

Note that we've replaced the partial derivatives on the right-hand side with total derivatives because they are derivatives of functions of a single variable. Substituting equations (21) and

(22) into equation (17) we get:

$$Y(x) \frac{d^2 T(t)}{dt^2} = c^2 T(t) \frac{d^2 Y(x)}{dx^2}$$

Note that the left-hand side of equation (23) is just a function of t and the right-hand side is only a function of x.

$$\frac{1}{c^2 T(t)} \frac{d^2 T(t)}{dt^2} = \frac{1}{Y(x)} \frac{d^2 Y(x)}{dx^2} \quad 2.23$$

This equation is also known as Klein Gordon Wave Equation. Now, comes the key step. It's simple, but you have to pay attention. How can a function of t, which in principle could be changing arbitrarily in time, be equal to a function of x that may be changing arbitrarily in space? Well, to make a long story short, the only way is if both sides of equation (23) are equal to the same constant which is called the separation constant.

For a reason that will become apparent later, let's let that constant be called $-k^2$, so:

$$\frac{1}{c^2 T(t)} \frac{d^2 T(t)}{dt^2} = -k^2$$

$$\frac{1}{Y(x)} \frac{d^2 Y(x)}{dx^2} = -k^2$$

which after a little rearranging can be rewritten as:

$$\frac{d^2 T(t)}{dt^2} = -k^2 c^2 T(t) = -\omega^2 T(t) \quad 2.24$$

$$\frac{d^2 Y(x)}{dx^2} = -k^2 Y(x) \quad 2.25$$

where the latter result in equation (25) holds because $\omega = ck$.

Equations (24) and (25) are the two ODEs whose solutions, Y (x) and T(t), can be substituted into equation (20) to give a solution to the PDE, the wave equation given by equation (17). Comparison of equations (24) and (25) with equation (6) reveals that both of these equations are simply Helmholtz equations, which we know how to solve because of their role in the SHO. Their solutions, therefore, are simply:

$$Y(x) = A \cos kx + B \sin kx \quad 2.26$$

$$T(t) = C \cos \omega t + D \sin \omega t \quad 2.27$$

where A;B;C; and D are arbitrary constants. You can see why we defined the separation constant as $-k^2$ because doing so yields equation (26) where k plays the role of wavenumber as we have defined it previously.

The boundary conditions allow us to find A as well as k and, hence, ω as we will now show. The initial conditions will specify the products BC and BD. This is discussed further in the next section.

Now, let's apply the boundary conditions. Assume that the string is clamped both at both ends: $x = 0$ and $x = a$. The boundary conditions, therefore, are $y(0; t) = y(a; t) = 0$ or equivalently $Y(0) = Y(a) = 0$, so using equations (26) and (27) we see that:

$$Y(0) = 0 = A\cos(0) + B\sin(0), \text{ so } A = 0 \quad 2.28$$

$$Y(a) = 0 = B\sin(ka), \text{ since } A \neq 0, \quad ka = n\pi \text{ or } k_n = \frac{n\pi}{a} \quad 2.29$$

where n is an integer. Remember that the expression $\sin^{-1}(0)$ should be read as the angle(s) at which sine is zero; which is just multiples of π .

We see, therefore, that we've established that there are a countable infinite number of allowable separation constants k indexed by the number n, that we recognize as the mode number or quantum number as discussed above. In section 1, we established that $k_n = \frac{n\pi}{a}$ based on purely physical considerations, here the reasoning was more mathematical but the result is the same. We see now that:

$$k_n = \frac{2\pi}{\lambda_n} = \frac{n\pi}{a} \text{ and } \omega_n = ck_n = \frac{n\pi c}{a} \quad 2.30$$

which is the same as equations (10) above. You can see through equations (28) and (29) how the boundary conditions determine the frequencies of oscillation in practice.

The final solution $y(x; t)$ is a linear combination of all of the solutions indexed by n:

$$\begin{aligned} y(x, t) &= \sum_n^\infty y_n(x, t) = \sum_n^\infty Y_n(x)T_n(t) \\ &= \sum_n^\infty B_n \sin k_x x [C_n \cos \omega_n t + D_n \sin \omega_n t] \end{aligned} \quad 2.31$$

$$\begin{aligned} &= \sum_n^\infty \sin k_x x [B_n C_n \cos \omega_n t + B_n D_n \sin \omega_n t] = \sum_n^\infty \sin k_x x [A'_n \cos \omega_n t + B'_n \sin \omega_n t] \\ y(x, t) &= \sum_n^\infty C'_n \sin k_x x [\sin(\omega_n t - \varphi_n)] \end{aligned} \quad 2.32$$

where we recombined the three arbitrary constants into two ($A'_n \equiv B_n C_n$ and $B'_n \equiv B_n D_n$) and also rewritten in terms of a phase shift φ_n which we will reference in the discussion of energy below. This reproduces the physically motivated equation (5) above. As before, the initial conditions will determine the coefficients (A'_n, B'_n) or (C_n, φ_n).

2.6. Application of Initial Conditions

For a string clamped at both ends, the solution for displacement $y(x; t)$, dropping the primes on the coefficients, is:

$$y(x, t) = \sum_{n=1}^{\infty} \sin k_n x [A_n \cos \omega t + B_n \sin \omega t] \quad 2.33$$

where the coefficients A_n and B_n depend on how the string is set into motion, i.e., on the initial conditions, and $k_n = \frac{n\pi}{L}$ and $\omega_n = c k_n$ where L is the length of the string and c is the speed of propagation of waves on the string.

If $f(x)$ and $g(x)$ are the initial patterns of displacement and velocity imparted to the string, then from equation (33) we see that:

$$y(x, 0) = f(x) = \sum_{n=1}^{\infty} A_n \sin k_n x = \sum_{n=1}^{\infty} a_n \sin k_n x \quad 2.34$$

$$v(x, 0) = \dot{y}(x, 0) = g(x) = \sum_{n=1}^{\infty} \omega_n B_n \sin k_n x = \sum_{n=1}^{\infty} b_n \sin k_n x \quad 2.35$$

The final equality in equations (34) and (35) is just the expansion of $f(x)$ and $g(x)$ in a Fourier Series. In both cases, the Fourier series is only a sine-series because the boundary conditions require that the function go to zero at the end-points ($x = 0$; $x = L$). As usual, the coefficients in the Fourier series are given by:

$$a_n = \frac{2}{L} \int_0^L f(x) \sin(k_n x) dx \quad 2.36$$

$$b_n = \frac{2}{L} \int_0^L g(x) \sin(k_n x) dx \quad 2.37$$

Here the constant in front of the integral is $2=L$ rather than $1=L$ because of interval we're considering goes from 0 to L rather than $-L=2$ to $L=2$. Comparison of equations (34) and (35) with (36) and (37) reveals that:

$$A_n = a_n = \frac{2}{L} \int_0^L f(x) \sin(k_n x) dx \quad 2.38$$

$$B_n = \frac{b_n}{\omega_n} = \frac{2}{\omega_n L} \int_0^L g(x) \sin(k_n x) dx \quad 2.39$$

These equations together with equation (33) give the solution to the problem with the initial conditions imposed.

Example: Let $y(x; 0) = f(x) = y_0 \sin(2\pi x/L)$ and $\dot{y}(x; 0) = g(x) = 0$. Then $a_n = y_0 \delta_{n2}$ and $b_n = 0$ so

$$y(x, t) = y_0 \sin\left(\frac{2\pi x}{L}\right) \cos\left(\frac{2\pi c t}{L}\right) \quad 2.40$$

CHAPTER 3

3. Blackbody Radiation

3.1 Blackbody: A quick review

Blackbody: An idealized model to study and understand the spectra of radiation emitted by a physical object or a body in thermal equilibrium maintained at temperature T . The ideal Blackbody is a good emitter and a good absorber of radiation irrespective of its shape, size, color or texture.

What is the problem: By 1870s, it was clear that light is part of a larger class called electromagnetic radiation (thanks to Maxwell's theory). The question arises as to what is the origin of electromagnetic radiation.

The pieces of Blackbody jigsaw: Experimental Blackbody results are shown in figure 1. The spectral energy density (energy content of Blackbody per unit volume in the frequency range between ν and $\nu + d\nu$) is plotted as a function of frequency ν . How can it be understood from theoretical considerations?

What's the use: Many bodies in nature are close approximations to an ideal Blackbody such as the Sun, earth and other heavenly bodies. The radiation from most objects on earth behaves as Blackbody radiation. Understanding the Blackbody radiation, among many other things, helps us to determine the temperature of the sun, other stars and planets, has implications for early universe and cosmology.

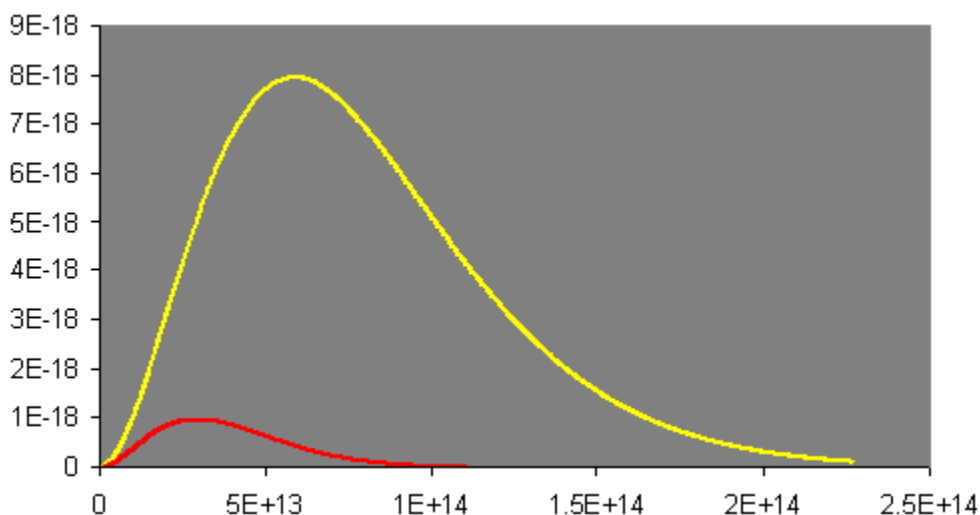


Figure 1: The spectral energy density $u(\nu).d\nu$ plotted as a function of frequency for two different temperatures.

3.2 The energy of a Blackbody

For the purposes of calculations, it is convenient to think of Blackbody as a cubic cavity of side L . A hole in one of the faces allows radiation to enter the cavity. Due to multiple reflections inside the cavity the radiation is nearly completely absorbed. Since the Blackbody is in equilibrium at temperature T , the energy content of the Blackbody is a constant except for small thermal fluctuations. This situation can be modelled by standing waves inside the Blackbody cavity.

Note that standing waves do not transmit any energy. This crucial idea is due to Lord Rayleigh who first attempted to explain the Blackbody spectrum 1890s. The total energy of the Blackbody is stored in the form of standing waves. The technique is to count the number of standing waves with frequencies in the range ν and $\nu + d\nu$. Thus, we have,

$$E(\nu)d\nu = N\bar{\epsilon}d\nu,$$

where N is the number of the standing waves and $\bar{\epsilon}$ is the average energy of each standing wave. Since we do not want our energy to be dependent on the volume of the cavity, we define energy density (energy per unit volume) in the frequency range ν and $\nu + d\nu$ to be,

$$u(\nu)d\nu = \frac{N}{L^3}\bar{\epsilon}d\nu \tag{3.1}$$

3.3 Number of standing waves

In principle, standing waves of all possible wavelengths should be present. However, the boundary conditions (waves should have a node at the walls of the cavity) of the cavity allow only modes of certain wavelengths to be present inside the cavity. The allowed wavelengths are obtained from the condition for standing waves in a cavity in one dimension to be $n = 2L/\lambda$, where λ is the wavelength of the standing wave and n is the number of half-wavelengths. In a 3D cavity, this condition is generalized to,

$$n_i = \frac{2L}{\lambda}, n_i = 1, 2, 3, \dots$$

Where i stands for the x, y, z cartesian coordinate for the three dimensional system. In 3D, each triplet of integers (n_x, n_y, n_z) correspond to a possible mode of standing wave inside the cavity. In a cube of side L , evidently the largest allowed standing wave will have a wavelength $2L$. This sets the upper limit for the allowed wavelengths or equivalently frequencies in the cavity.

The number of standing waves above a given value of wavelength, say $\bar{\lambda}$, is the number of such triplets (or modes) which have wavelengths above $\bar{\lambda}$. There is an easier and approximate way to calculate this quantity. Consider a 3D space of integers (n_x, n_y, n_z) and every point in this space corresponds to one possible mode of standing wave. Since there are large number of modes, we can concern this space as being essentially continuous and ask how many independent modes lie in the range of wavelengths λ and $\lambda + d\lambda$. This is given by the surface area of a shell in one octant of sphere as (where octant (or solid geometry) is one of the 8 divisions of the 3-D space by coordinate planes, see figure 2)

$$2 \left(\frac{1}{8}\right) 4\pi n^2 dn \tag{3.2}$$

The factor 2 comes from two possible states of polarisation for each standing wave. We want the result in terms of frequency and so we write n in terms of frequency as,

$$n = \frac{2L}{\lambda} = \frac{2Lv}{c} \text{ and } dn = \frac{2L}{c} dv \quad 3.3$$

Substituting for n from Eq. 3 in Eq. 2 we get the result for number of standing waves in the cavity in $[v, v + dv]$ to be,

$$\text{Number of standing waves in } (v, v + dv) = 8\pi L^3/c^3 v^2 dv \quad 3.4$$

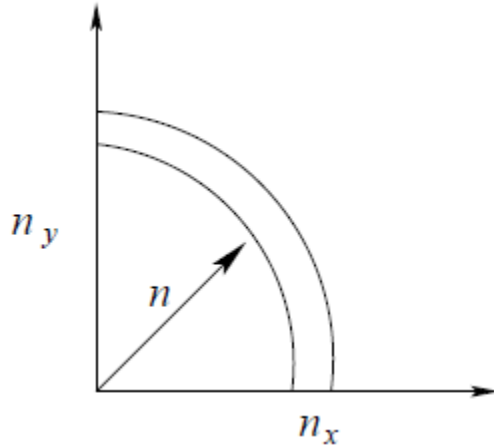


Figure 2: Number of standing waves in the frequency range $[v, v + dv]$. We should determine the number of points in the shell of radius n . However, if the points are close enough we can simply assume them to be continuous and calculate the area of the shell.

3.4 Average energy

The other factor we need to compute the energy density that is the average energy of each mode of standing wave. Classically, this is obtained from the theorem of equipartition of energy which states that for systems in equilibrium at temperature T , the energy associated with each degree of freedom is $kT/2$, where k is the Boltzmann constant. Physically, the standing waves inside the cavity arise from harmonic oscillations of the electrons in the walls of the cavity. From the point of view of equipartition theorem, harmonic oscillator has two degrees of freedom (one potential and one kinetic) and hence the average energy is $\bar{\epsilon} = kT$.

3.5 Rayleigh-Jeans formula

Substituting all the known values in Eq. 1, we get the required energy density to be,

$$u(\nu)d\nu = \frac{8\pi\nu^2}{c^3}kTd\nu \quad 3.5$$

This is the Rayleigh-Jeans formula. The obvious problem with this relation is that the total energy integrated from $\nu = 0$ to $\nu = 1$ gives infinity. This is unphysical and clearly not supported by experimental results shown in fig 1.

3.6 Wien approximation

Wien's approximation (also sometimes called **Wien's law** or the **Wien distribution law**) is a law of physics used to describe the spectrum of thermal radiation (frequently called the blackbody function). This law was first derived by Wilhelm Wien in 1896. The equation does accurately describe the short wavelength (or high frequency) spectrum of thermal emission from objects, but it fails to accurately fit the experimental data for long wavelengths (low frequency) emission.

Wien derived his law from thermodynamic arguments, several years before Planck introduced the quantization of radiation. The law may be written as

$$u(\nu, T) = \frac{2h\nu^3}{c^2} e^{-h\nu/kT} \quad 3.6$$

Where $u(\nu, T)$ is the amount of energy per unit surface area per unit time per unit solid angle per unit frequency emitted at a frequency ν , T is the temperature of the Blackbody, h is Planck's constant, c is the speed of light and k is Boltzmann's constant.

This equation may also be written as

$$u(\lambda, T) = \frac{2hc^2}{\lambda^5} e^{-hc/\lambda kT} \quad 3.7$$

where $u(\lambda, T)$ is the amount of energy per unit surface area per unit time per unit solid angle per unit wavelength emitted at a wavelength λ .

3.7 Wien's displacement law

Wien's displacement law shows how the spectrum of black-body radiation at any temperature is related to the spectrum at any other temperature. If we know the shape of the spectrum at one temperature, we can calculate the shape at any other temperature. Spectral intensity can be expressed as a function of wavelength or of frequency.

A consequence of Wien's displacement law is that the wavelength at which the intensity *per unit wavelength* of the radiation produced by a Blackbody is at a maximum, λ_{\max} , is a function only of the temperature

The peak value of this curve, as determined by taking the derivative and solving for zero, occurs at a wavelength λ_{\max} and frequency ν_{\max} of:

$$\lambda_{\max} \cdot T = b \quad 3.8$$

where the constant, b , known as Wien's displacement constant, is equal to $2.8977721(26) \times 10^{-3}$ K m.

3.8 Planck's radiation law

Max Planck assumed that the energy exchange between the oscillators on the walls of the cavity and the standing waves takes place in discrete quanta given by,

$$E_n = nh\nu \quad 3.9$$

where h is the Planck's constant. Using this energy relation in Boltzmann distribution, $f(E) = \exp(-E/kT)$, he obtained the average energy to be,

$$\bar{\epsilon} = \frac{h\nu}{[e^{h\nu/kT} - 1]} \quad 3.10$$

$$u(\nu)d\nu = \left(\frac{8\pi h}{c^3}\right) \frac{\nu^3 d\nu}{[e^{h\nu/kT} - 1]} \quad 3.11$$

This is the Planck's radiation law and displays excellent agreement with the measured Blackbody spectrum. In the limit, $\nu \rightarrow \infty$, we recover the Rayleigh-Jeans law as in Eq. 5.

Exercise : Calculate the average energy using Boltzmann distribution if the energy formula is $E_n = nh\nu$. The result is given in Eq. 10.

3.9 Power radiated by a Blackbody

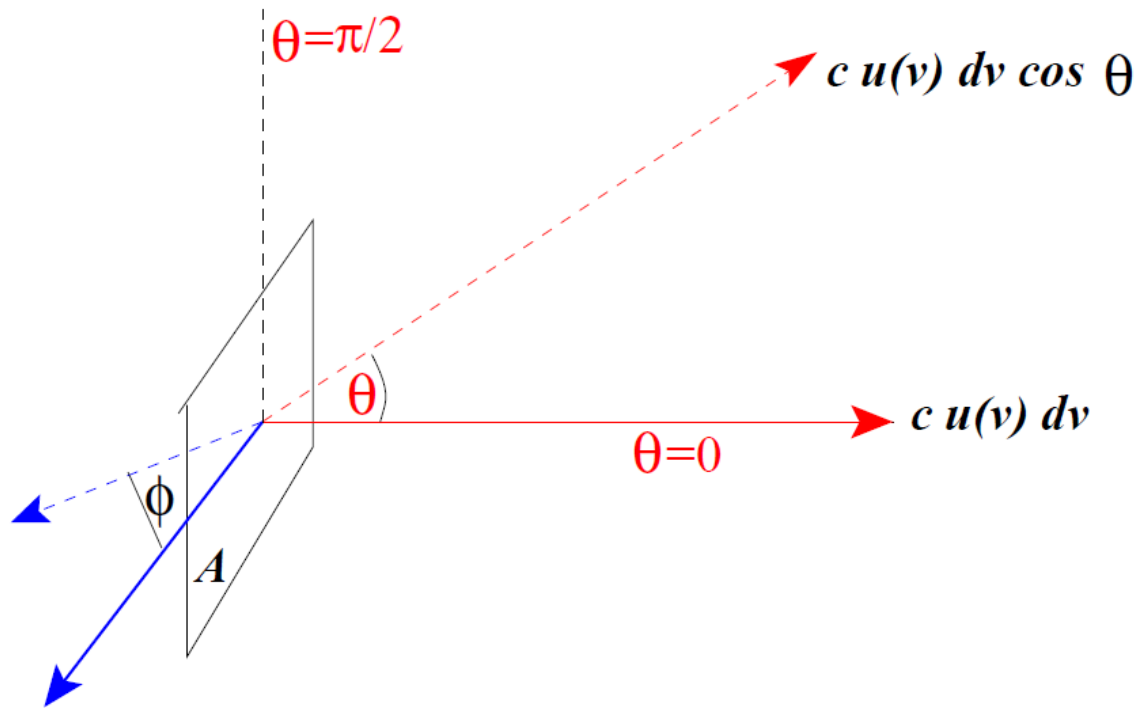


Figure 3: The power emitted by face A of the imaginary cube will spread itself out in the entire hemisphere defined by $0 \leq \theta \leq \pi/2$, $0 \leq \phi \leq 2\pi$. The directions corresponding to $\theta = 0$ and $\theta = \pi/2$ are marked in the figure.

Power, by definition, is the energy transmitted per second. For the Blackbody, we will calculate the power transferred by a Blackbody per second per unit area. We will start from the energy density $u(\nu) d\nu$ in the frequency range $[\nu, \nu + d\nu]$. Consider a unit cube radiating outwards in all possible directions. Actually, as shown in Fig 3, we are interested in calculating the power radiated by the face A of the cube. Radiation emitted per unit area is the energy per unit volume (energy density) divided by the distance the radiation travels in time dt . It is given by

$$u(\nu) d\nu c dt$$

Power radiated (energy transferred per unit time) per unit area is

$$u(\nu) d\nu c.$$

This energy is radiated out in all possible directions, i.e, in all 4π solid angle. The power radiated in solid angle $d\Omega$ is given by,

$$u(\nu) d\nu c \frac{d\Omega}{4\pi}$$

Now, while doing this, irrespective of the shape of the Blackbody, we are implicitly accounting only for the radiation coming out of unit surface area in a given direction. The

radiation going out on other directions appears to be ignored in this calculation but would be accounted for when power radiated by the entire surface of Blackbody is calculated.

Next, the radiation emerging from unit area of the Blackbody surface will go out in all the directions in the hemisphere. Thus, the emerging radiation, in general, makes an angle θ with respect to the normal on the unit surface. Then, the power emitted in solid angle $d\Omega$ is,

$$u(\nu) d\nu \frac{d\Omega}{4\pi} \cos\theta$$

An area element for solid angle d is given by,

$$d\Omega = \sin\theta \, d\theta \, d\phi, \quad 0 \leq \theta \leq \pi/2, \quad 0 \leq \phi \leq 2\pi.$$

Now, the power emitted in to a solid angle d is given by,

$$u(\nu) d\nu \frac{c}{4\pi} \cos\theta \sin\theta \, d\theta \, d\phi,$$

Now, the total power emitted per unit area of the black surface in the frequency range $[\nu, \nu+d\nu]$ is simply the integral of the power emitted in to the entire hemisphere. Thus, we get,

Substituting from Eq. 11 and doing the integrals, the final result is,

$$P(\nu) d\nu = u(\nu) d\nu \frac{c}{4\pi} \int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi/2} \cos\theta \sin\theta \, d\theta \, d\phi$$

$$P(\nu) d\nu = u(\nu) d\nu \frac{c}{4\pi} \left[\frac{1}{2} \sin^2\theta \right]_0^{\pi/2} [\phi]_0^{2\pi} = \left(\frac{c}{4} \right) u(\nu) d\nu \quad 3.12$$

Substituting from eq. 8 and doing the integrals, the final results is,

$$P(\nu) d\nu = \frac{2\pi h}{c^2} \frac{\nu^3}{[e^{h\nu/kT} - 1]} d\nu \quad 3.13$$

This is the power radiated per unit area in frequency range $[\nu, \nu + d\nu]$. By integrating over ν , the total power radiated in all the frequencies can be obtained. This gives the well-known Stefan Boltzmann law.

Exercise : Obtain an expression for Stefan-Boltzmann constant starting from Eq. 13.

Exercise : Calculate the power received by the planet Mars from the sun. And calculate the average temperature on the surface of Mars. Compare it with the measured temperature of Mars and explain the discrepancy, if any.

3.10 Relation of Planck's law to the Wien approximation

The Wien approximation was originally proposed as a description of the complete spectrum of thermal radiation, although it failed to accurately describe long wavelength (low frequency) emission. However, it was soon superseded by Planck's law, developed by Max Planck.

Unlike the Wien approximation, Planck's law accurately describes the complete spectrum of thermal radiation. Planck's law may be given as

$$P(\nu, T)d\nu = \frac{2\pi h}{c^2} \frac{\nu^3}{[e^{h\nu/kT}-1]} d\nu \quad 3.13$$

The Wien approximation may be derived from Planck's law by assuming $h\nu \gg kT$. When this is true, then

$$\frac{1}{e^{h\nu/kT}-1} \approx e^{-h\nu/kT}$$

and so Planck's law approximately equals the Wien approximation at high frequencies.

3.11 Stefan–Boltzmann Law

The Stefan–Boltzmann law states that the power emitted per unit area of the surface of a Blackbody is directly proportional to the fourth power of its absolute temperature:

$$P = \sigma T^4 \quad 3.14$$

$$j^* = \sigma T^4, \quad 3.15$$

where j^* is the total power radiated per unit area, T is the absolute temperature and $\sigma = 5.67 \times 10^{-8} \text{ W m}^{-2} \text{ K}^{-4}$ is the Stefan–Boltzmann constant. This follows from integrating over $u(\nu, T)$ frequency and solid angle:

$$P = \int_0^\infty d\nu \int d\Omega \cos\theta. u(\nu, T) \quad 3.16$$

The $\cos\theta$ factor appears since we are considering the radiation in the direction normal to the surface. The solid angle integral extends over the full 2π in azimuth ϕ , and over half the domain of polar angle θ :

$$\int d\Omega \cos\theta = \int_{\phi=0}^{2\pi} d\phi \int_{\theta=0}^{\pi/2} \cos\theta \sin\theta d\theta = \pi \quad 3.17$$

$u(\nu, T)$ is independent of angles and passes through the solid angle integral. Inserting the formula for $u(\nu, T)$ gives

$$P = \frac{2\pi(kT)^4}{(ch)^3} \int_0^\infty \frac{x^3}{e^x-1} dx \quad 3.18$$

where $x = h\nu/kT$ is unitless. The integral over x has the value: $\int_0^\infty \frac{x^3}{e^x - 1} dx = \frac{\pi^4}{15}$, which gives

$$P = \sigma \cdot T^4 \quad 3.19$$

$$\sigma = \frac{2\pi^5 k^4}{15(ch)^3} \quad 3.20$$

3.12 Human body emission

As all matter, the human body radiates some of a person's energy away as infrared light.

The net power radiated is the difference between the power emitted and the power absorbed:

$$P_{net} = P_{emit} - P_{absorb} \quad 3.21$$

Applying the Stefan–Boltzmann law,

$$P_{net} = A\sigma\epsilon \cdot (T^4 - T_0^4) \quad 3.21$$

The total surface area of an adult is about 2 m², and the mid- and far-infrared emissivity of skin and most clothing is near unity, as it is for most nonmetallic surfaces. Skin temperature is about 33 °C, but clothing reduces the surface temperature to about 28 °C when the ambient temperature is 20 °C. Hence, the net radiative heat loss is about

$$P_{net} = A\sigma\epsilon \cdot (T^4 - T_0^4) = 100 \text{ W} \quad 3.22$$

The total energy radiated in one day is about 9 MJ (mega joules), or 2000 kcal (food calories).

Basal metabolic rate for a 40-year-old male is about 35 kcal/(m²·h), which is equivalent to 1700 kcal per day assuming the same 2 m² area. However, the mean metabolic rate of sedentary adults is about 50% to 70% greater than their basal rate.

There are other important thermal loss mechanisms, including convection and evaporation. Conduction is negligible – the Nusselt number is much greater than unity. Evaporation via perspiration is only required if radiation and convection are insufficient to maintain a steady state temperature (but evaporation from the lungs occurs regardless). Free convection rates are comparable, albeit somewhat lower, than radiative rates. Thus, radiation accounts for about two-thirds of thermal energy loss in cool, still air. Given the approximate nature of many of the assumptions, this can only be taken as a crude estimate. Ambient air motion, causing

forced convection, or evaporation reduces the relative importance of radiation as a thermal loss mechanism.

Application of Wien's Law to human body emission results in a peak wavelength of

$$\lambda_{\max} = \frac{2.898 \times 10^{-3} \text{ K.m}}{305 \text{ K}} = 9.50 \text{ } \mu\text{m} \quad 3.23$$

For this reason, thermal imaging devices for human subjects are most sensitive in the 7–14 micron range.

3.13 Appendix

The Nusselt Number

For forced convection of a single-phase fluid with moderate temperature differences, the heat flux per unit area q_{ω}^H is nearly proportional to the temperature difference $\Delta T = T_{\omega} - T_{*}$. This was discovered by Newton who then inferred that $q_{\omega}^H \sim \Delta T$. Thus we arrive at Newton's law of cooling:

$$q_{\omega}^H = h(T_{\omega} - T_{*})$$

where h is called the heat transfer coefficient, with units of $\frac{W}{m^2}$. But h is dimensional and thus its value depends on the units used. The traditional dimensionless form of h is the **Nusselt number Nu**, which may be defined as the ratio of convection heat transfer to fluid conduction heat transfer under the same conditions. Consider a layer of fluid of width L and temperature difference $T_{\omega} - T_{*}$. Assuming that the layer is moving so that convection occurs, the heat flux would be,

$$q_{\omega}^H = h(T_{\omega} - T_{*})$$

If, on the other hand, the layer were stagnant, the heat flux would be entirely due to fluid conduction through the layer:

$$q_{\omega}^H = \frac{k(T_{\omega} - T_{*})}{L}$$

We define the Nusselt number as the ratio of these two:

$$N_{UL} = \frac{q_{\omega}^{II}(\text{Convective heat transfer})}{q_{\omega}^{II}(\text{Conductive heat transfer})} = \frac{hL}{k}$$

A Nusselt number of order unity would indicate a sluggish motion little more effective than pure fluid conduction: for example, laminar flow in a long pipe. A large Nusselt number means very efficient convection: For example, turbulent pipe flow yields N_{UL} of order 100 to 1000.

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