

# Classical Mechanics, what we need for?

MECHANICS, OSCILLATOR, WAVES

Surprisingly, many concepts from the classical mechanics remain valid in quantum mechanics, such as: **kinetic energy, momentum, potential energy, force...** 

Fundamentals of Quantum Mechanics for Materials Scientists



**Newtonian** classical mechanics VS **Hamiltonian** CM: same physics but different mathematical approaches

We will mainly deal with the non-relativistic quantum mechanics: any particles with mass must effectively be moving much slower than the velocity of light.

P.S. Photons do have to travel at the velocity of light, but they have no mass...we can still avoid to explicitly include he relativistic effects for most of the physic of photons.

Fundamentals of Quantum Mechanics for Materials Scientists



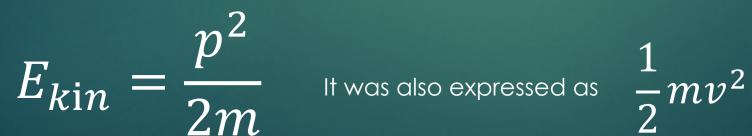
# Momentum and kinetic energy

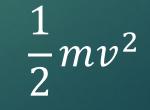
**Classical momentum** for a particle of mass **m** 

 $\boldsymbol{p} = m \boldsymbol{v}$ 

It is a vector, because it has a direction.

The kinetic energy for the motion is:





Fundamentals of Quantum Mechanics for Materials Scientists



# Momentum and kinetic energy

The kinetic energy for the motion is:

 $E_{kin} = \frac{p^2}{2m}$ 

where

 $p^2 \equiv \boldsymbol{p} \cdot \boldsymbol{p}$ 

The vector dot product of **p** with itself

Fundamentals of Quantum Mechanics for Materials Scientists

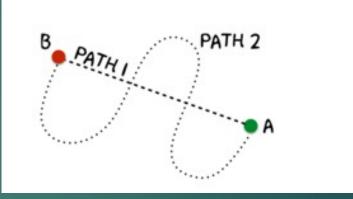
# Potential energy



It is the energy due to position and typically denoted by V in QM. Not to be confused with the voltage!

Can be written as: V(r)

r is the vector position



Potential energy depends only on the position (where the particle is), not about the path (how it got there).

Fundamentals of Quantum Mechanics for Materials Scientists

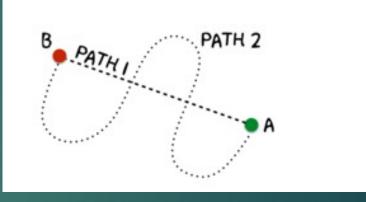
# Potential energy



Potential energy depends only on the position (where the particle is), not about the path (how it got there).

Fields with this property are called **CONSERVATIVE** 

The change in potential energy going around any **closed path**, e.g., PATH 1+PATH 2 is **zero**.



Good examples are gravitational fields and electrostatic fields. Some other fields are not conservative, e.g., frictional force.

Fundamentals of Quantum Mechanics for Materials Scientists

# Total Energy energy



It is the sum of potential and kinetic energy.

When written as a function of position and momentum, it can be called classical Hamiltonian.

Thus, for a classical particle with mass m in a conservative potential V(r), the Hamiltonian will be:

$$H = \frac{p^2}{2m} + V(r)$$



In quantum mechanics, we rarely use the force directly as in the Newton's law.

We can express the same idea by thinking of a force as the **gradient of the potential energy**. We will use these potentials in QM, instead of the forces directly.

 $\Delta V = -F\Delta x$ 

Thus:  $F = -\frac{\Delta V}{\Delta x}$ 

Fundamentals of Quantum Mechanics for Materials Scientists

 $F \longrightarrow a \longrightarrow b \times V(a) \qquad V(b)$ 





In quantum mechanics, we rarely use the force directly as in the Newton's law.

We can express the same idea by thinking of a force as the **gradient** of the potential energy. We will use these potentials in QM, instead of the forces directly.

 $\Delta V = -F\Delta x$ 

Thus:  $F = -\frac{\Delta V}{\Delta x}$ 

Fundamentals of Quantum Mechanics for Materials Scientists

Why negative?

F in the definition of potential energy is the force exerted by the force field, e.g., gravity, spring force, etc. The potential energy V is equal to the work you must do against that force ...



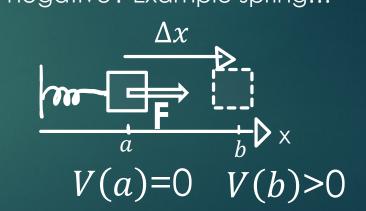
In quantum mechanics, we rarely use the force directly as in the Newton's law.

We can express the same idea by thinking of a force as the **gradient** of the potential energy. We will use these potentials in QM, instead of the forces directly. <u>Why negative? Example spring...</u>

 $\Delta V = -F\Delta x$ 

Thus:  $F = -\frac{\Delta V}{\Delta x}$ 

Fundamentals of Quantum Mechanics for Materials Scientists



 $\Delta V = -(-K\Delta x)\Delta x$ 



In the limit of infinitesimal  $\Delta x$  :

 $F = -\frac{\mathrm{d}V}{\mathrm{d}x}$ 

we can generalize our idea of the relation between potential and force to three dimensions, with force as a vector, by using the gradient operator:

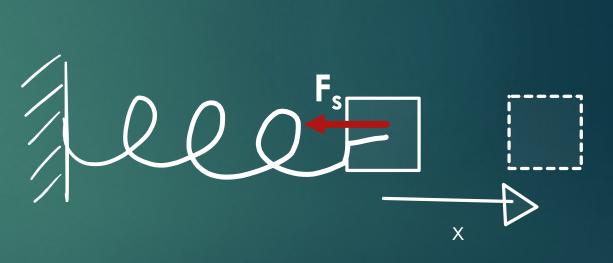
$$\bar{F} = -\nabla V \equiv -\left[\frac{\delta V}{\delta x}\mathbf{i} + \frac{\delta V}{\delta y}\mathbf{j} + \frac{\delta V}{\delta z}\mathbf{k}\right]$$

Fundamentals of Quantum Mechanics for Materials Scientists

# Harmonic Oscillator

The spring will act a restoring force  $F_S$  on the mass M proportional to the displacement x, with K the spring constant.

$$F_S = -Kx$$



The minus sign is because of the restoring force trying to pull the mass back and resetting x to 0. This will create a simple **harmonic oscillator**.

Fundamentals of Quantum Mechanics for Materials Scientists



#### Harmonic Oscillator

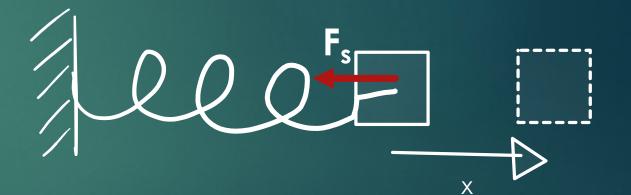


$$F_S = Ma = M\frac{\mathrm{d}^2 x}{\mathrm{d}t^2} = -Kx$$

So: 
$$\frac{\mathrm{d}^2 x}{\mathrm{d}t^2} = -\frac{K}{M}x = -\omega^2 x$$

We define

 $\omega^2 = \frac{K}{M}$ 



Fundamentals of Quantum Mechanics for Materials Scientists

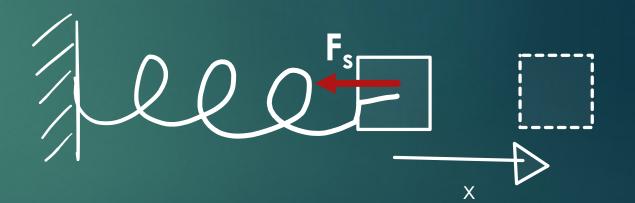
### Harmonic Oscillator



So: 
$$\frac{\mathrm{d}^2 x}{\mathrm{d}t^2} = -\frac{k}{M}x = -\omega^2 x$$

We define 
$$\omega^2 = \frac{\kappa}{M}$$

We have solutions like  $x \propto \sin \omega t$ 



With 
$$\omega=\sqrt{k/M}$$
 angular freq  $\omega=2\pi f$ 

Fundamentals of Quantum Mechanics for Materials Scientists

# Simple harmonic oscillator



# It is a physical system described by the equation: $\frac{d^2x}{dt^2} = -\omega^2 x$

Many examples:

- Spring systems (and not just the simple classical one)
- Electrical resonator
- Acoustic resonators
- Linear oscillators (in general)

Fundamentals of Quantum Mechanics for Materials Scientists

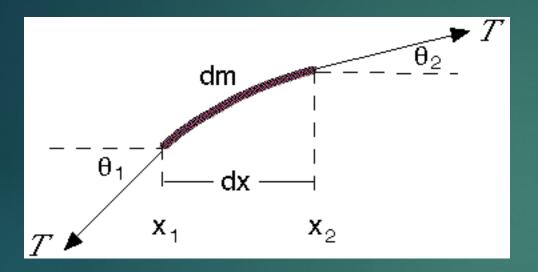


Plucking the guitar strings, they make notes...

We're going to be looking at the equation that describes waves on a string, and therefore, how you get the different notes.

Fundamentals of Quantum Mechanics for Materials Scientists





The diagram shows a short section of a string, stretched in the x direction, and the forces acting on it. It is stretched by a tension *T*, and its equilibrium position is along the x axis. This small section have a mass dm and will experience vertical displacement along y axis.

Fundamentals of Quantum Mechanics for Materials Scientists

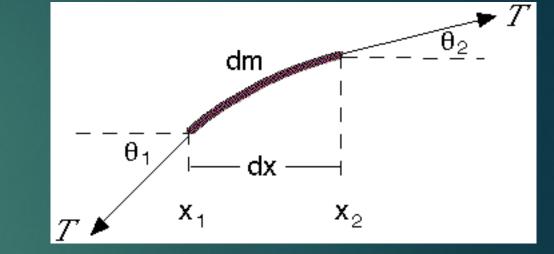


A force  $T \sin \theta_2$  pulls mass dm upwards A force  $T \sin \theta_1$  pulls mass dm downwards

The sum of forces in the y direction is  $F_y = T \sin \theta_2 - T \sin \theta_1$ .

Using the small angle approximation, sin  $\theta \cong \tan \theta = \frac{\partial y}{\partial x}$ . So we may write:  $F_{y} = T\left(\frac{\delta y}{\delta x}\right)_{2} - T\left(\frac{\delta y}{\delta x}\right)_{1}$ 





The total force depends on the difference **in slope between** the two ends: if the string were straight, the two forces would add up to zero (for any slope).

Fundamentals of Quantum Mechanics for Materials Scientists

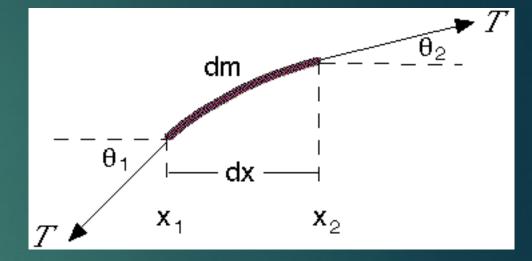
 $F_{y} = T\left(\left(\frac{\delta y}{\delta x}\right)_{2} - \left(\frac{\delta y}{\delta x}\right)_{1}\right)$ 



Considering a mass per unit length is  $\rho$ dm =  $\rho$  dx

By applying second newtons law:  $F_{y} = ma_{y}$ but, we can wrie  $a_{y} = \frac{\partial v_{y}}{\partial t} = \frac{\partial y^{2}}{\partial t^{2}}.$ Thus:

$$F_{y} = T\left(\left(\frac{\delta y}{\delta x}\right)_{2} - \left(\frac{\delta y}{\delta x}\right)_{1}\right) = \rho \, \mathrm{dx} \, \frac{\delta^{2} y}{\delta t^{2}}$$

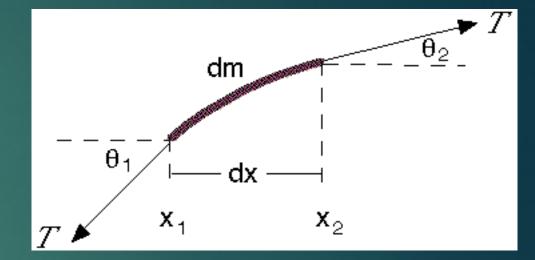


Fundamentals of Quantum Mechanics for Materials Scientists

$$F_{y} = T\left(\left(\frac{\delta y}{\delta x}\right)_{2} - \left(\frac{\delta y}{\delta x}\right)_{1}\right) = \rho \, \mathrm{dx} \, \frac{\delta^{2} y}{\delta t^{2}}$$

Rearranging it:

$$\frac{\delta^2 y}{\delta t^2} = \frac{T}{\rho} \frac{\left(\frac{\delta y}{\delta x}\right)_2 - \left(\frac{\delta y}{\delta x}\right)_1}{dx}$$



Because the last term expresses the change in first derivative between  $x_1$  and  $x_{2,1}$  it correspond to the second derivative...we get:

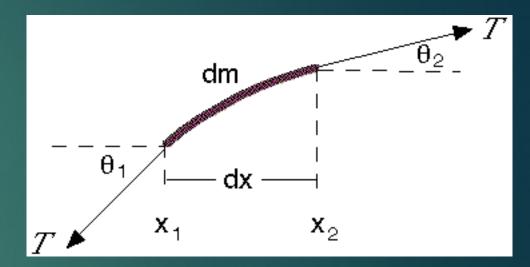
$$\frac{\delta^2 y}{\delta t^2} = \frac{T}{\rho} \frac{\delta^2 y}{\delta x^2}$$

Fundamentals of Quantum Mechanics for Materials Scientists





 $\frac{\delta^2 y}{\delta t^2} = \frac{T}{\rho} \frac{\delta^2 y}{\delta x^2}$ If  $v^2 = \frac{T}{\rho}$  we will get:



 $\frac{\delta^2 y}{\delta t^2} - v^2 \frac{\delta^2 y}{\delta x^2} = 0$ 

Which is a classical wave equation for a wave with velocity :

Fundamentals of Quantum Mechanics for Materials Scientists

 $v = \sqrt{\frac{7}{4}}$ 



$$\frac{\delta^2 y}{\delta t^2} - \nu^2 \frac{\delta^2 y}{\delta x^2} = 0$$

General solutions are functions like: f(x - vt) which is a wave travelling to the right at speed v

Fundamentals of Quantum Mechanics for Materials Scientists



$$\frac{\delta^2 y}{\delta t^2} - \nu^2 \frac{\delta^2 y}{\delta x^2} = 0$$

Similarly, we could have functions like: g(x + vt) which is a wave travelling to the left at speed v

Fundamentals of Quantum Mechanics for Materials Scientists



Often, we work with waves travelling at the light velocity c, thus:

$$\frac{\delta^2 y}{\delta t^2} - c^2 \frac{\delta^2 y}{\delta x^2} = 0 \quad \text{with} \quad f(x \pm ct)$$

Often, we're interested in waves that are oscillating at one specific angular frequency  $\omega$ , thus we've got a temporal behaviour of this form (or any combination of these):

$$T(t) = e^{i\omega t}, e^{-i\omega t}, \cos(\omega t), \sin(\omega t)$$

Fundamentals of Quantum Mechanics for Materials Scientists



Often, we work with waves travelling at the light velocity c, thus:

$$\frac{\delta^2 y}{\delta t^2} - c^2 \frac{\delta^2 y}{\delta x^2} = 0 \qquad \text{with} \qquad f(x - ct)$$

Temporal behaviour of this form (or any combination of these):  $T(t) = e^{i\omega t}, e^{-i\omega t}, \cos(\omega t), \sin(\omega t)$ 

We can write a solution of the wave equation as some product of the variation in x times the variation in t:

$$\phi(x,t) = X(x)T(t)$$

Fundamentals of Quantum Mechanics for Materials Scientists

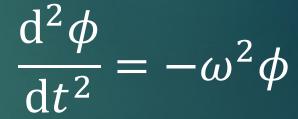


Temporal behaviour of this form (or any combination of these):

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

We can write a solution of the wave equation as some product of the variation in x times the variation in t:

```
\phi(x,t) = X(x)T(t) And we will have
```



That we can put back into the wave equation:

$$\frac{\delta^2 \phi}{\delta t^2} - c^2 \, \frac{\delta^2 \phi}{\delta x^2} = 0$$

Obtaining:  $c^2 \frac{\delta^2 \phi}{\delta r^2} + \omega^2 \phi = 0$ 

Fundamentals of Quantum Mechanics for Materials Scientists



Temporal behaviour of this form (or any combination of these):

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

We can write a solution of the wave equation as some product of the variation in x times the variation in t:

$$\phi(x,t) = X(x)T(t)$$
 And we will have

$$\frac{\mathrm{d}^2\phi}{\mathrm{d}t^2} = -\omega^2\phi$$

Thus the remaining spatial part equation is:

$$\frac{d^{2}X(x)}{dx^{2}} + k^{2}X(x) = 0 \text{ with } k^{2} = \frac{\omega^{2}}{c^{2}}$$

Fundamentals of Quantum Mechanics for Materials Scientists



# The remaining spatial part equation is: $\frac{d^2 X(x)}{dx^2} + k^2 X(x) = 0 \quad \text{with}$



This is working if we have only one frequency (monochromatic wave). A simple version of the general expression for a sine wave travelling in the positive x direction is:

$$\phi = A\sin(kx - \omega t)$$

Fundamentals of Quantum Mechanics for Materials Scientists

emilio.scalise@unimib.it

 $k^2 = \frac{\omega^2}{c^2}$ 



The remaining spatial part equation is:  $\frac{\mathrm{d}^2 X(x)}{\mathrm{d}x^2} + k^2 X(x) = 0 \quad \text{with} \qquad k^2 = \frac{\omega^2}{c^2}$ 

Temporal part:

$$\frac{\mathrm{d}^2\phi}{\mathrm{d}t^2} = -\omega^2\phi$$

General solution:  $\phi = A \sin(kx - \omega t)$ 

Fundamentals of Quantum Mechanics for Materials Scientists

# Standing waves



A combination of waves travelling one to the right and one to the left is:

$$\phi(\mathbf{x}, \mathbf{t}) = \sin(kx - \omega t) + \sin(kx + \omega t)$$
  
$$\equiv 2\cos(\omega t) \sin(kx)$$

This gives a standing waves, because it is always the same shape in space.



Fundamentals of Quantum Mechanics for Materials Scientists

