The Single-Electron Problem in Quantum Mechanics

a. Electron in a one-dimensional potential box.

In quantum mechanics, the **particle in a box** model (also known as the **infinite potential well** or the **infinite square well**) describes a particle free to move in a small space surrounded by impenetrable barriers. The model is mainly used as a hypothetical example to illustrate the differences between classical and quantum systems.

One-dimensional solution

The simplest form of the particle in a box model considers a one-dimensional system. Here, the particle may only move backwards and forwards along a straight line with impenetrable barriers at either end.[1] The walls of a one-dimensional box may be visualised as regions of space with an infinitely large potential energy. Conversely, the interior of the box has a constant, zero potential energy.[2] This means that no forces act upon the particle inside the box and it can move freely in that region. However, infinitely large forces repel the particle if it touches the walls of the box, preventing it from escaping. The potential energy in this model is given as

$$V(x) = \begin{cases} 0, & 0 < x < L, \\ \infty, & \text{otherwise}, \end{cases},$$

where L is the length of the box and x is the position of the particle within the box.

n quantum mechanics, the wavefunction gives the most fundamental description of the behavior of a particle; the measurable properties of the particle (such as its position, momentum and energy) may all be derived from the wavefunction.[3] The wavefunction $\psi(x,t)$ can be found by solving the Schrödinger equation. Inside the box, no forces act upon the particle, which means that the part of the wavefunction inside the box oscillates through space and time with the same form as a free particle:[1][4]

$$\psi(x,t) = [A\sin(kx) + B\cos(kx)]\mathrm{e}^{-i\omega t},$$

where A and B are arbitrary complex numbers. The frequency of the oscillations through space and time are given by the wavenumber k and the angular frequency ω respectively. These are both related to the total energy of the particle by the expression

$$E = \hbar\omega = \frac{\hbar^2 k^2}{2m},$$

which is known as the dispersion relation for a free particle.

b. Electron in a one-dimensional harmonic oscillator

Harmonic oscillator = potential energy depends on square of the space coordinate- force (-gradient of the potential) has a linear dependence on the coordinate.
Many symmetric "potential wells" can be approximated by harmonic oscillator potentia close to the potential minimum (lowest order in the Taylor expansion which is symmetric for negative-positive coordinate.)
Thus many physical problems which involve small oscillations of the system not too far from equilibrium are approximated by harmonic oscillator.
Out of many examples: oscillations of "electron clouds" of atoms "provoked" by electromagnetic fields or temperature , molecules, electromagnetic fields itself etc etc

etc etc.

$$H(p,q)=\frac{p^2}{2m}+\frac{1}{2}m\omega^2 q^2$$

$$U=\frac{1}{2}m\omega^2 q^2, \quad F=-dU/dq=-m\omega^2 q \stackrel{\text{def}}{=} -kq \rightarrow k=m\omega^2$$

$$E_{pot}(x)=\frac{1}{2}C\cdot x^2; \qquad \omega=\sqrt{\frac{C}{m}};$$

$$E_n=\hbar\omega(n+\frac{1}{2}), \quad n=0,1,2,\ldots$$

c. Electron in a three-dimensional potential box. Electron in a cubic box. Electron in a quantum well; quantum line and quantum dot.

Let us explore the workings of wave mechanics in three dimensions through the example of a particle confined to a cubic "box." The box has edge length L and occupies the region 0 < a, b, c < L. We assume the walls of the box are smooth, so they exert forces only perpendicular to the surface, and that collisions with the walls are elastic. A classical particle would rattle around inside such a box, colliding with the walls. At each collision, the component of particle momentum normal to the wall is reversed (changes sign), while the other two components of momentum are unaffected.

A Ψ hullámfüggvény meghatározásához meg kell oldanunk a Schrödinger-egyenletet, amit továbbra is a változók szétválasztása módszerrel tehetünk meg legkönyebben, hisz ekkor tudjuk, hogy

$$\Psi(\mathbf{r},t) = \Psi(\mathbf{r})\phi(t),$$

és

$$\phi(t) = e^{-j\frac{E}{\hbar}t}.$$

Mielőtt azonban rátérnék a $\Psi(\boldsymbol{r})$ meghatározására, adjuk meg a konfigurációs téren a potenciált:

$$E_{pot}(\mathbf{r}) = \begin{cases} 0 & \text{ha x} \in (0,a),\ \text{y} \in (0,b),\ \text{z} \in (0,c) \\ \infty & \text{különben} \end{cases}$$

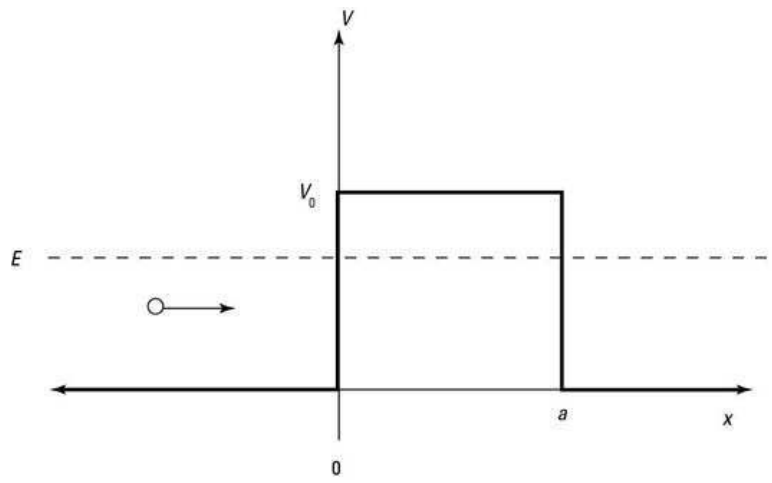
Innetől csak az időfüggetlen Schrödinger-egyenletet kell megoldanunk, ami a következő:

$$\mathbf{H}\Psi = -\frac{\hbar^2}{2m}\triangle\Psi = E\Psi.$$

A változók szétválasztása módszerrel az alábbi energia képletet kapjuk:

$$E_{n_1 n_2 n_3} = \frac{h^2}{8ma^2}(n_1^2 + n_2^2 + n_3^2), \quad n_1, n_2, n_3 = 1, 2, \ldots$$

d.



Transmission of a particle through a potential barrier (quantum tunneling)

When a particle doesn't have as much energy as the potential of a barrier, you can use the Schrödinger equation to find the probability that the particle will tunnel through the barrier's potential. You can also find the reflection and transmission coefficients, R and T, as well as calculate the transmission coefficient using the *Wentzel-Kramers-Brillouin* (WKB) approximation.
Here's how it works: When a particle doesn't have as much energy as the potential of the barrier, you're facing the situation shown in the following figure

A potential barrier $E < V_0$.

In this case, the Schrödinger equation looks like this:

- **For the region $x < 0$:** $\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}$

- **For the region $0 < x < a$:** $\frac{d^2\psi_2}{dx^2}(x) - k_2^2\psi(x) = 0$

  where $k_2^2 = \frac{2m(V_0 - E)}{\hbar^2}$

- **For the region $x > a$:** $\frac{d^2\psi_3(x)}{dx^2} + k_1^2\psi_3(x) = 0$

  where $k_1^2 = \frac{2mE}{\hbar^2}$.

All this means that the solutions for

$\psi_1(x)$, $\psi_2(x)$, *and* $\psi_3(x)$

are the following:

- **Where $x < 0$:** $\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}$
- **For the region $0 < x < a$:** $\psi_2(x) = Ce^{k_2x} + De^{-k_2x}$
- **Where $x > a$:** $\psi_3(x) = Fe^{ik_1x} + Ge^{-ik_1x}$

  In fact, there's no leftward traveling wave in the region $x > a$; $G = 0$,

  so $\psi_3(x)$ is $\psi_3(x) = Fe^{ik_1x}$.

This situation is similar to the case where $E > V_0$, except for the region

$0 \le x \le a$.

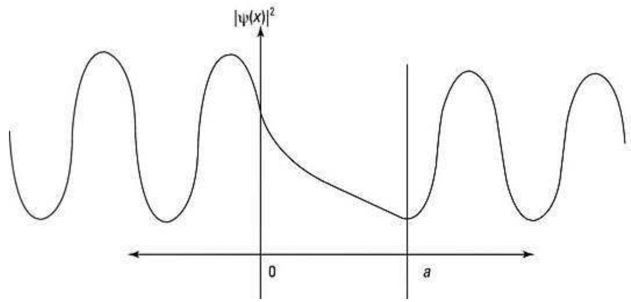
The wave function oscillates in the regions where it has positive energy, $x < 0$ and $x > a$, but is a decaying exponential in the region

$0 \le x \le a$.

You can see what the probability density,

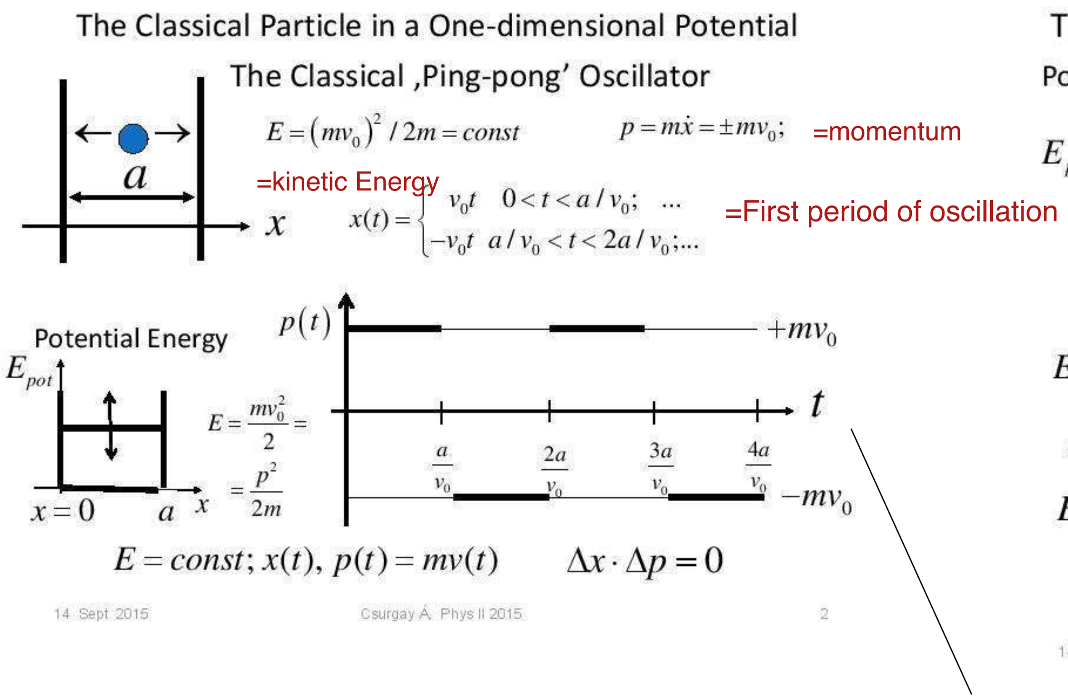
$|\psi(x)|^2$,

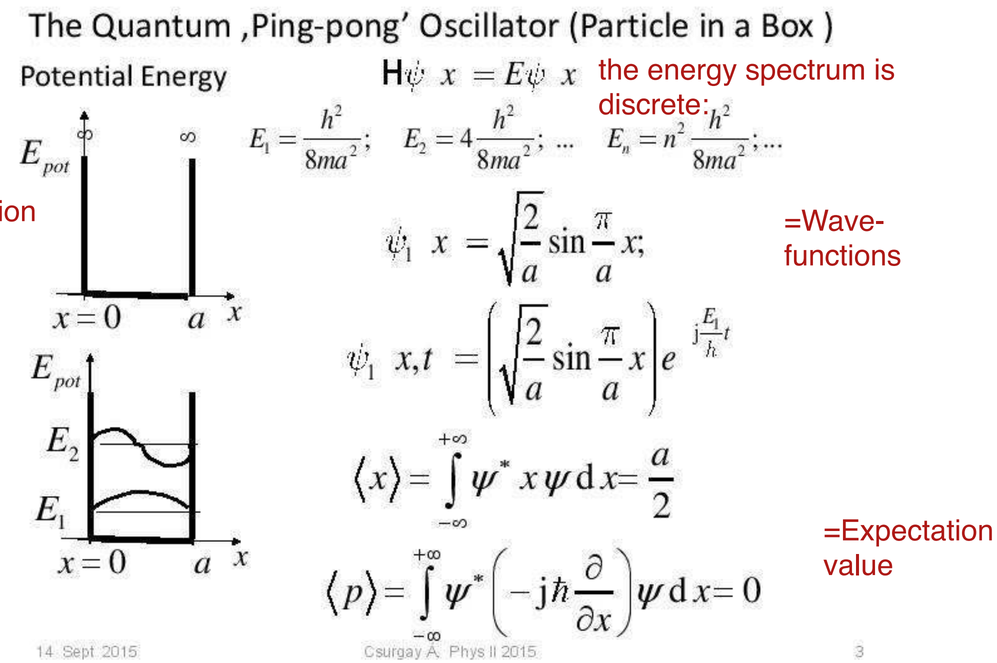
looks like in the following figure.



e. The classical and quantum ping-pong oscillator

We have seen that a monochromatic electromagnetic field as a cavity mode is mathematically equivalent to a quantum mechanical harmonic oscillator of the same resonant frequency. First, let us recall the classical one-dimensional oscillators. The simplest oscillator is the classical 'ping-pong' ball. Let us initiate the ping-pong dynamics by an initial velocity v0.

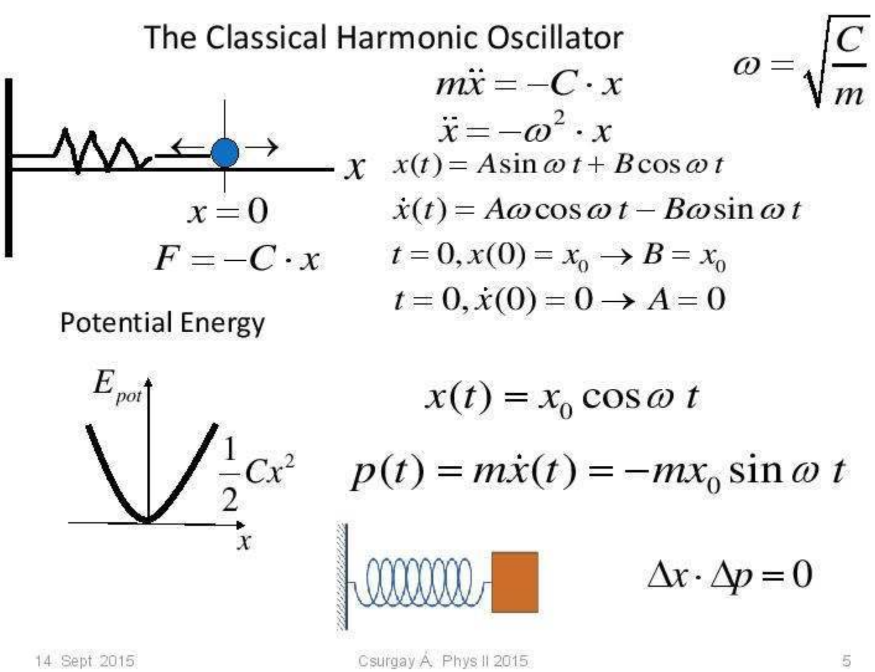


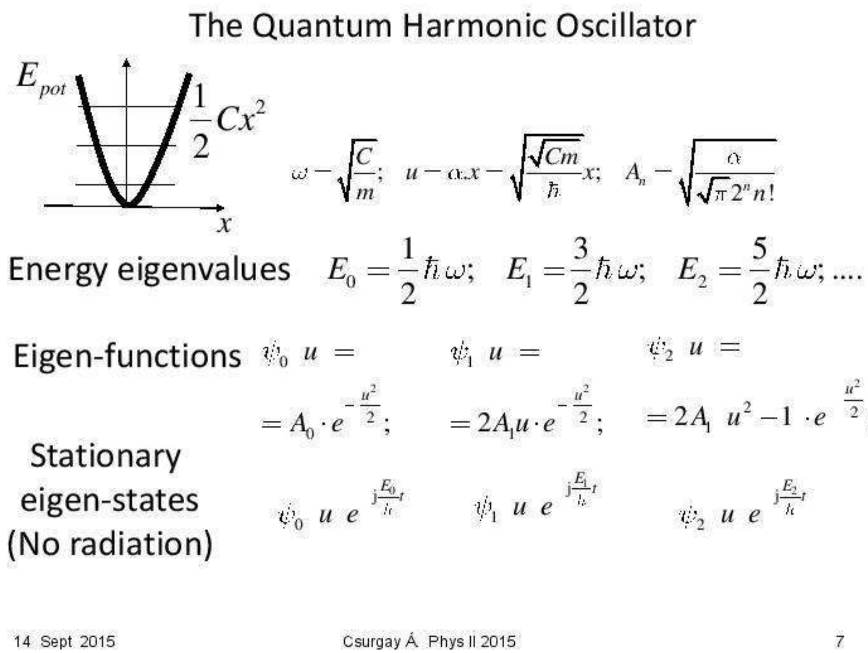


The potential Energy and the p(t) momentum as a function of time

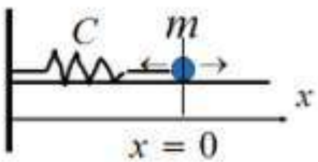
Note that the constant energy can be changed continuously by changing the initial velocity v0.

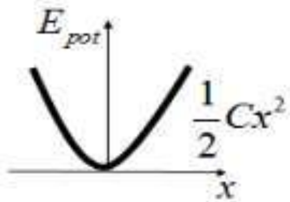
f. The classical and quantum harmonic oscillator





In a classical mechanical one-dimensional harmonic oscillator a mass m is oscillating the end of a string, characterized by its constant, C. The position of the mass is x, its at momentum is $p = m \cdot \dot{x}$. The kinetic energy of the mass is $p^2 / 2m$, and the potential energy of the string is $C \cdot x^2 / 2$. The resonant frequency is $\omega = \sqrt{C / m}$. The Lagrangian is $L = p^2 / 2m - m\omega^2 q / 2$, and the Hamiltonian is $H = p^2 / 2m + m\omega^2 q / 2$.





The classical Hamilton equations of motion are: $\dot{x} = p / m;\ \dot{p} = -m\omega^2 x$. If at $t = 0$ we pull (or push) the string to position x_0, then the dynamics will be $x(t) = x_0 \cos \omega t$ and the momentum is $p(t) = m\dot{x}(t) = -mx_0 \sin \omega t$. The the accuracy of the simultaneous measurement of the position and momentum can be accurate, i.e. the product of the variances can approach zero without any theoretical limit $\Delta x \cdot \Delta p \to 0$.

In case of the harmonic oscillator, the eigen-values and eigenunctions have been derived as:

$E_n = \hbar\omega(n + \frac{1}{2}),\quad n = 0,1,2,\ldots,\qquad \psi_n \ x = A_n \varphi_n(u) \cdot e^{-\frac{u^2}{2}}$ where

$\omega = \sqrt{\frac{C}{m}};\quad u = \alpha . x = \sqrt{\frac{\sqrt{Cm}}{\hbar}} x;\quad A_n = \sqrt{\frac{\alpha}{\sqrt{\pi} 2^n n!}}$, and

$\varphi_0(u) = 1;\quad \varphi_1(u) = 2u;\quad \varphi_2(u) = 4u^2 - 2$ are Hermite polynomials.