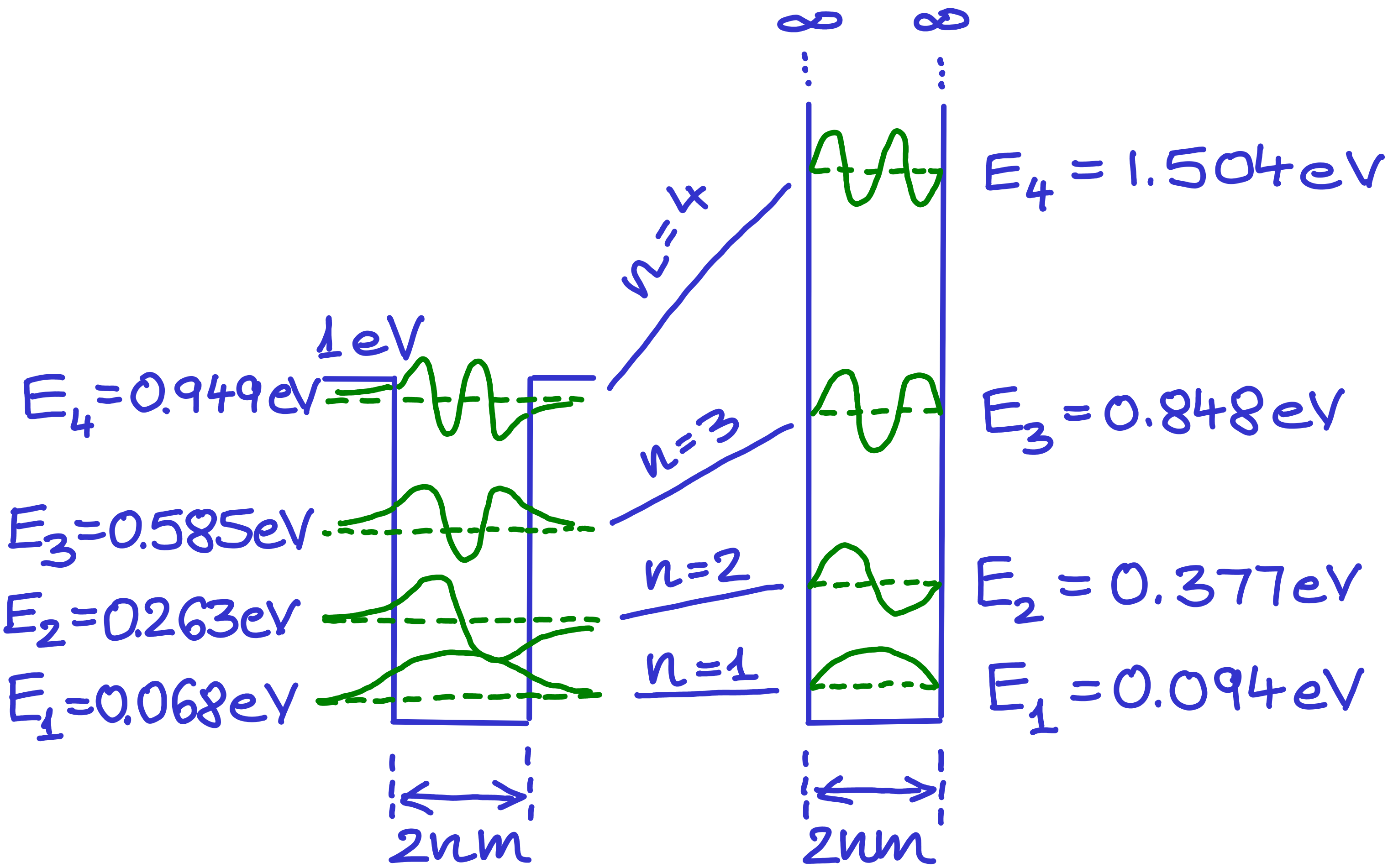
Finite versus infinite square well



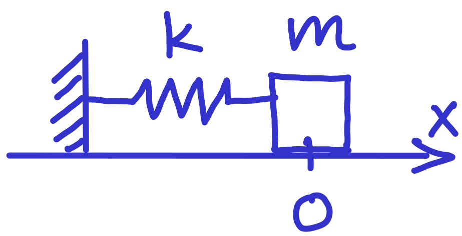
$L = 2\,nm$; particle: electron: $m_e = 511\,\frac{keV}{c^2}$

$$E_{n,\infty} = n^2 \cdot \frac{h^2}{8mL^2} = n^2 \cdot \frac{h^2c^2}{8mc^2L^2}$$

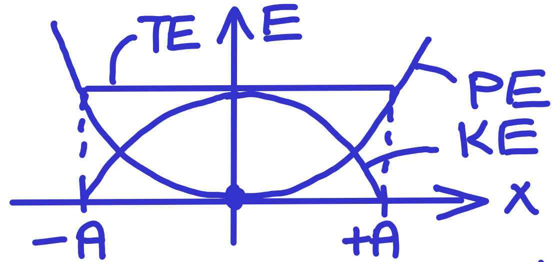
An infinite potential well has infinite number of states, a finite potential well has finite number of states. The states represent bound states. If the well gets very shallow, it can have only one or even zero bound states.

[Deuteron (p-n) has one state only.]

Simple harmonic oscillator



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



$PE = \frac{1}{2} k x^2$; $KE = \frac{1}{2} m v^2$; $TE = KE + PE$: const.

(H)—WW—(H) : chemical bonds can be modelled very well as oscillators.

$$-\frac{\hbar^2}{2m} \cdot \frac{d^2\psi(x)}{dx^2} + \frac{1}{2} k x^2 \cdot \psi(x) = E\psi(x)$$

$$\frac{1}{2} k x_0^2 = \frac{1}{2}\hbar\omega \Rightarrow x_0 = \sqrt{\frac{\hbar\omega}{k}} = \sqrt{\frac{\hbar}{m\omega}}$$

$$k = m\omega^2$$

x_0 : classical turning point, if

$$TE = E = \frac{1}{2}\hbar\omega = E_0$$

New variable (without unit):

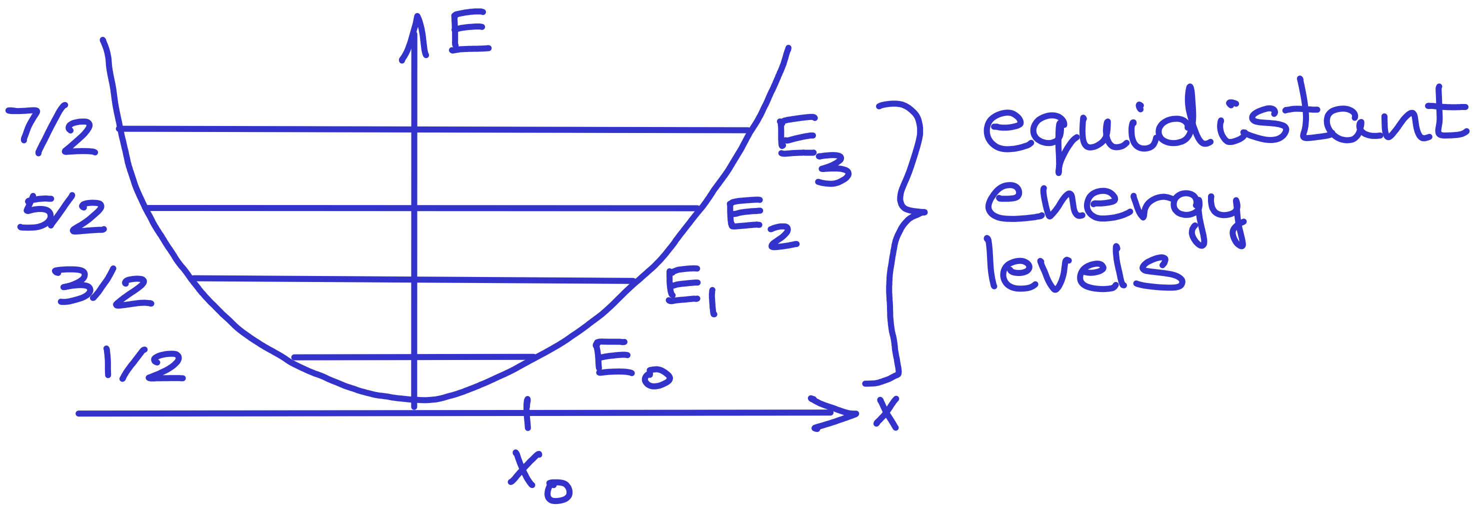
$$\xi = \frac{x}{x_0} = \sqrt{\frac{m\omega}{\hbar}} \cdot x = \sqrt{\frac{k}{\hbar\omega}} \cdot x$$

$$\psi_n(\xi) = \underbrace{\frac{1}{\sqrt{2^n \cdot n! \sqrt{\pi} \cdot x_0}}}_{\text{normalization factor}} \cdot \underbrace{H_n(\xi)}_{\text{Hermite polynomial}} \cdot \underbrace{e^{-\frac{1}{2}\xi^2}}_{\text{Gaussian}}$$

Simple harmonic oscillator 2.

Energy of the oscillator:

$$\boxed{E_n = \left(\frac{1}{2}+n\right)\hbar\omega = \left(\frac{1}{2}+n\right)hf \qquad n=0,1,2,3,\ldots}$$



Hermite polynomials:

$$H_0(\xi) = 1$$

$$H_1(\xi) = 2\xi$$

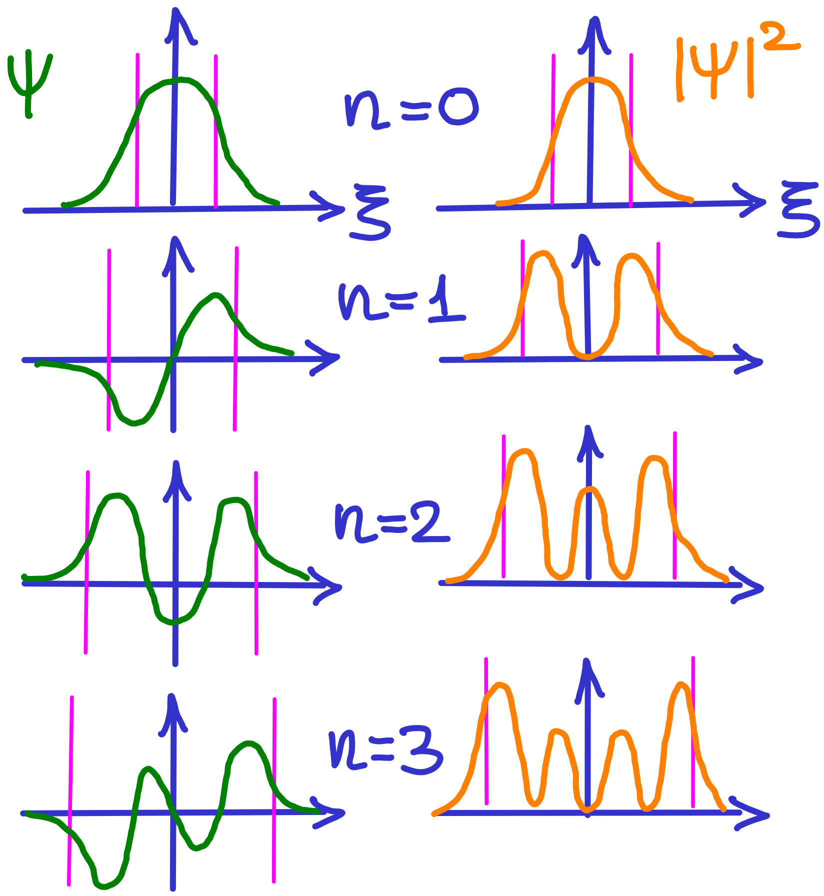
$$H_2(\xi) = 4\xi^2 - 2$$

$$H_3(\xi) = 8\xi^3 - 12\xi$$

$$H_4(\xi) = 16\xi^4 - 48\xi^2 + 12$$

$$H_5(\xi) = 32\xi^5 - 160\xi^3 + 120\xi$$

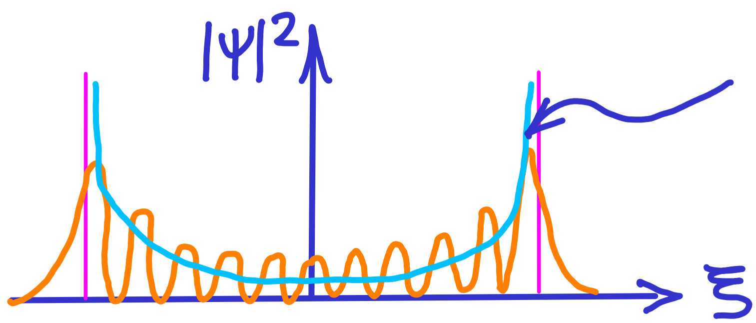
Simple harmonic oscillator 3.



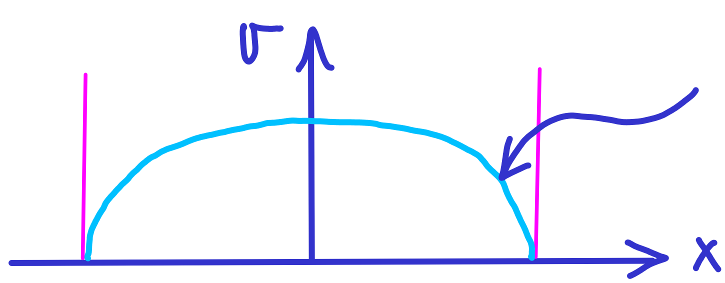
The correspondence principle:

Quantum mechanical results must reduce to classical physics results in the limit of large quantum numbers (or, more generally, when systems become large or energies become high compared to quantum scales).

It was proposed by Bohr in 1913.



classical probability $\sim \frac{1}{v}$



$$\frac{1}{2}kx^2 + \frac{1}{2}mv^2 = E$$

(ellipse)

Correspondance Principle: ☑