QM II.

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SZÉCHENYI ISTVÁN EGYETEM
SZE - GYŐR

Fizika és Kémia Tanszék

Quantum harmonic oscillator

Total energy of the mass point oscillating harmonicly:

$$E = \frac{p^2}{2m} + \frac{1}{2}Dx^2$$

Since the total energy (thus the Hamiltonian) is independent of time, we have to solve the stationary Schrödinger equation.

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It can be written in the next form:

$$\left\{-\frac{\hbar^2}{2m}\Delta + V(x,y,z)\right\}\Psi(x,y,z) = E\Psi(x,y,z)$$

$$\hat{H}\Psi(x,y,z) = E\Psi(x,y,z)$$

So the stationary Schrödinger equation is actually the eigenvalue equation of the time-independent Hamiltonian operator!

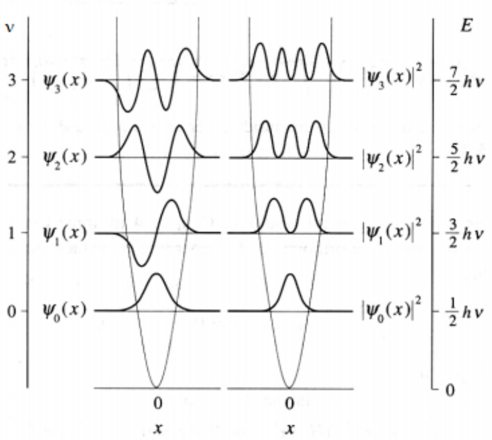
The solution of the previous eigenvalue equation for the Hamiltonian operator of harmonic oscillations is:

$$E_\nu = \left(\nu + \frac{1}{2}\right)\hbar\sqrt{\frac{D}{m}} = \left(\nu + \frac{1}{2}\right)\hbar\omega_0$$

$$\psi_\nu(x) = e^{-\frac{\xi^2}{2}} H_\nu(\xi), \quad \xi = \sqrt{\frac{m\omega_0}{\hbar}}x$$

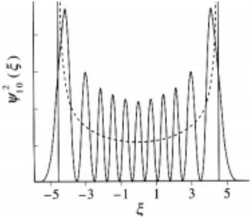
ν – vibrational quantum number

Again, we see that the zero-point energy of the system is a positive, non-zero value!



v
3
2
1
0
$\psi_3(x)$
$\psi_2(x)$
$\psi_1(x)$
$\psi_0(x)$
$|\psi_3(x)|^2$
$|\psi_2(x)|^2$
$|\psi_1(x)|^2$
$|\psi_0(x)|^2$
E
$\frac{7}{2}h\nu$
$\frac{5}{2}h\nu$
$\frac{3}{2}h\nu$
$\frac{1}{2}h\nu$
0
0
x
0
x

$\nu = 10$



$\psi_{10}^2(\xi)$
−5
−3
−1
1
3
5
ξ

Equation of continuity

Schrödinger equation:

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Multiply the first equation by Ψ^*, while the second by $(-\Psi)$, and after summing up these two equations:

$$-\frac{\hbar^2}{2m}\left\{\Psi^*\Delta\Psi - \Psi\Delta\Psi^*\right\} = i\hbar\frac{\partial\Psi^*\Psi}{\partial t}$$

After rearrangement:

$$\frac{\partial \Psi^* \Psi}{\partial t} + \frac{\hbar}{2im}\left\{\Psi \Delta \Psi^* - \Psi^* \Delta \Psi\right\} = 0$$

We know that $\Delta f = div\ grad\ f$,thus:

$$\Psi \Delta \Psi^* - \Psi^* \Delta \Psi = \Psi div\ grad\ \Psi^* - \Psi^* div\ grad\ \Psi =$$

$$= div\left(\Psi grad\ \Psi^* - \Psi^* grad\ \Psi\right)$$

Let us introduce next notations:

$$\rho = \Psi^* \Psi, \quad \underline{j} = \frac{\hbar}{2im}\left(\Psi grad\ \Psi^* - \Psi^* grad\ \Psi\right).$$

The equation of continuity for quantum probability is:

$$\frac{\partial \rho}{\partial t} + div \underline{j} = 0$$

ρ-probability density, $\underline{j}$-current density of probability

Tunnel–effect

Let an electron approaches a potential step with a certain kinetic energy E_k. We only deal with the case when the kinetic energy of the electron in the classical sense is not enough to overcome the potential, i.e. $E_k < V$.

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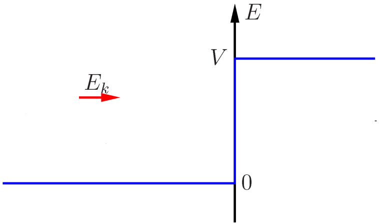

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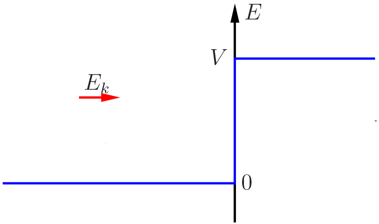

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Total energy of the particle:

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Due to the jump of the potential at the origin, the equation must be solved separately on the negative and positive sides of the x-axis.

$x < 0$, $E_p = 0$. So here the equation to be solved is:

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Let's find the solution of this equation in the following form:

$$\varphi_n(x) = e^{ik_0x} + Ae^{-ik_0x}.$$

Here $i = \sqrt{-1}$ is the imaginary unit.

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Physical meaning: a plane wave of unit amplitude approaches the potential step + after reflection, a reflected plane wave of amplitude A also contributes to the solution.

$x \geq 0$, $E_p = V$. So here the equation to be solved is:

$$\frac{d^2\varphi_p(x)}{dx^2} + \frac{2m(E - V)}{\hbar^2}\varphi_p(x) = 0.$$

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In this particular case the expression $\frac{2m(E-V)}{\hbar^2}$ is negative, because $E < V$. Let us introduce notion $-K^2 = \frac{2m(E-V)}{\hbar^2}$. The equation takes the following form:

$$\frac{d^2\varphi_p(x)}{dx^2} - K^2\varphi_p(x) = 0,$$

or what is the same:

$$\frac{d^2\varphi_p(x)}{dx^2} = K^2\varphi_p(x).$$

Let us find the solution in the following form:

$$\varphi_p(x) = Ce^{-Kx} + De^{Kx}.$$

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The height of the potential step is finite at the point $x = 0$, the obtained solutions and their first derivatives (due to the continuity equation, the probability density current must be continuous at $x = 0$) must be identical on the both sides of $x = 0$. Therefore:

$$1 + A = C$$

$$ik_0(1 - A) = -KC$$

Solving this system of equations, we get:

$$A = \frac{ik_0 + K}{ik_0 - K},$$

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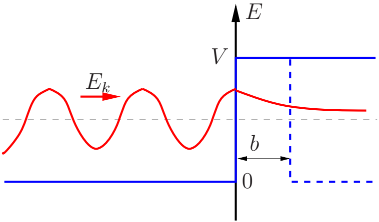
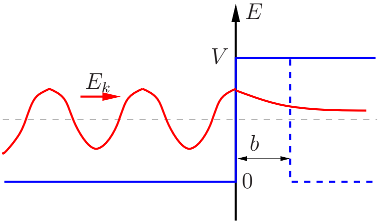
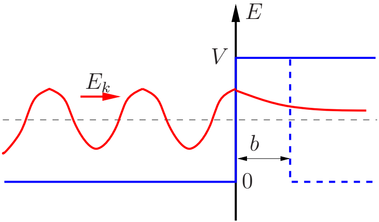
We can say that the electron also penetrates the region inaccessible to it in the classical sense.


E
V
E_k
b
0



If the potential step has a finite width, then the electron can pass through this classically inaccesible region. The probability of passing through (T) is proportional to the following quantity:

$$T \sim \frac{\varphi_p^2(b)}{\varphi_p^2(0)} \sim e^{-\frac{2b}{\hbar}\sqrt{2m(V-E)}}$$



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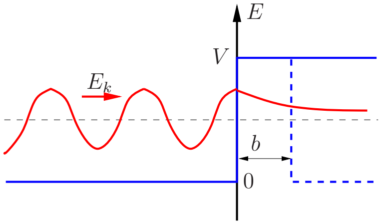
$\boldsymbol{T}$ is decreasing if $\boldsymbol{b}$ is increasing, or if $\boldsymbol{V-E}$ is increasing.



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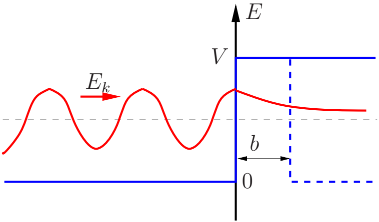

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