PHY 530
STEEM Refresher course 1
introduction to quantum mechanics

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INSTITUT PHOTOVOLTAÏQUE D'ILE-DE-FRANCE

UMR 9006

STEEM Refresher 1

1. Reminder on thermodynamics
2. Introducing quantum mechanics postulate
3. (Tutorial) Application to the flat potential well – eigen states
4. (Tutorial) Application to the flat potential well – quantum rules
5. (Tutorial) Application to the flat potential well – double well
6. Conclusion & take home message

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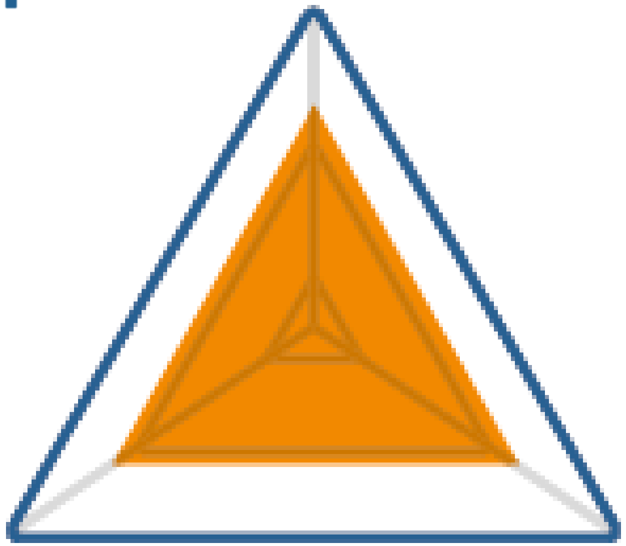
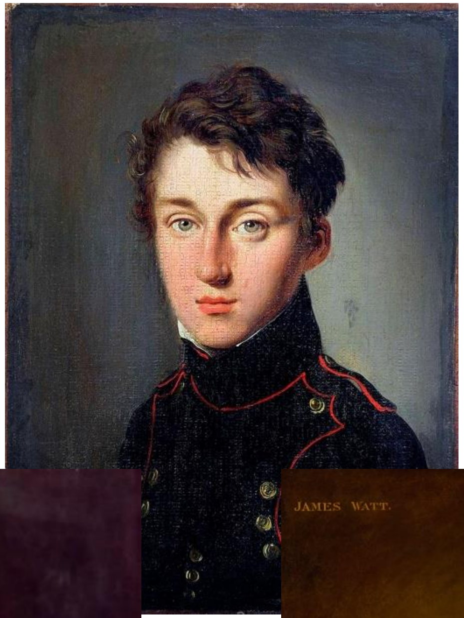
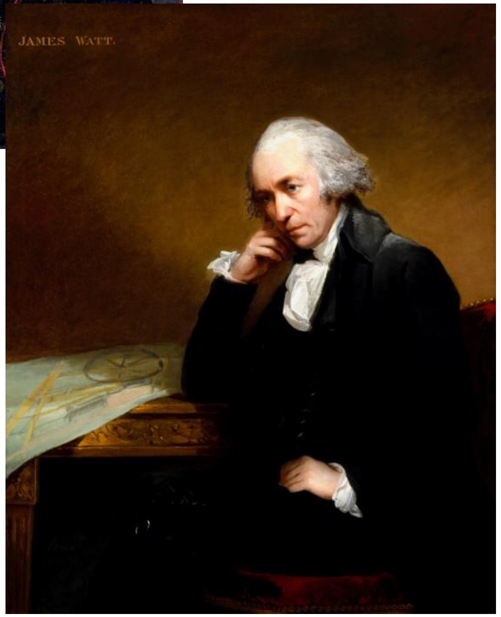
Energy ?

WORLD
ENERGY
COUNCIL







First law of thermodynamics

Energy now = energy before + energy input – energy output

H. Callen, Thermodynamics and an introduction to thermostatistics

Properly speaking, energy is never created or consumed – only exchanged

Energy can be exchanged through heat or work

$$\Delta E = W + Q$$

Energy Work Heat

Heat and work are two ways to exchange energy. A system *does not contains* heat or work, it contains energy.

Second law of thermodynamics

Entropy can not be destroyed

(Entropy measures the disorder of a system, but we don't care here)

$$dS = \delta S_{\text{exch.}} + \delta S_{\text{crea.}}$$

$\delta S_{\text{exch.}} \to \frac{\delta Q}{T_{\text{ext}}}$ $\qquad \delta S_{\text{crea.}} \geq 0$

- If some heat gets in, some heat *must* get out

$\Delta U = 0 = W + Q_{in} - Q_{out}$

Over a cycle : $\Delta S = S_f - S_i = 0$

- To produce work, it is not sufficient to have heat. Cold is also needed

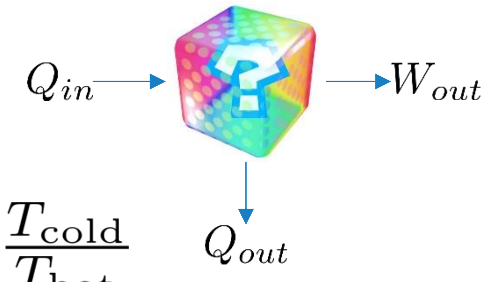
$$T_{\text{out}} = T_{\text{in}} \Rightarrow Q_{\text{out}} \geq Q_{\text{in}} \Rightarrow W \leq 0$$

$$S_{\text{crea.}} = -\frac{Q_{\text{in}}}{T_{\text{in}}} + \frac{Q_{\text{out}}}{T_{\text{out}}} \geq 0$$

$= -S_{exch}$

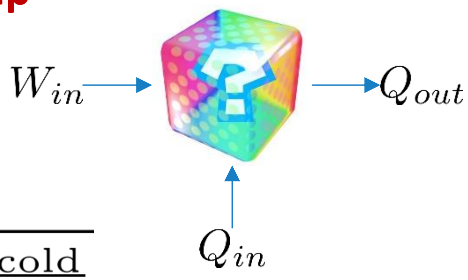
$\left(\frac{Q_{in}}{T_{in}} - \frac{Q_{out}}{T_{out}}\right)$

Engine



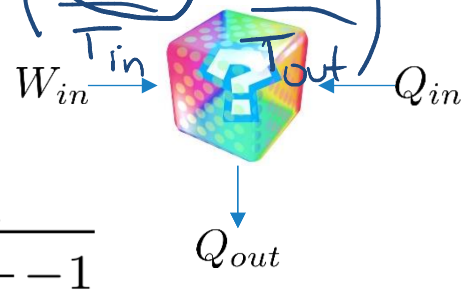
$$\eta = 1 - \frac{T_{\text{cold}}}{T_{\text{hot}}}$$

Heat pump



$$\eta = \frac{1}{1 - \frac{T_{\text{cold}}}{T_{\text{hot}}}}$$

Fridge



$$\eta = \frac{1}{\frac{T_{\text{hot}}}{T_{\text{cold}}} - 1}$$

A brief history of thermodynamics

RÉFLEXIONS

SUR LA

PUISSANCE MOTRICE

DU FEU

ET

SUR LES MACHINES

PROPRES A DÉVELOPPER CETTE PUISSANCE.

PAR S. CARNOT,

ANCIEN ÉLÈVE DE L'ÉCOLE POLYTECHNIQUE.

A PARIS,

CHEZ BACHELIER, LIBRAIRE,

QUAI DES AUGUSTINS, N°. 55.

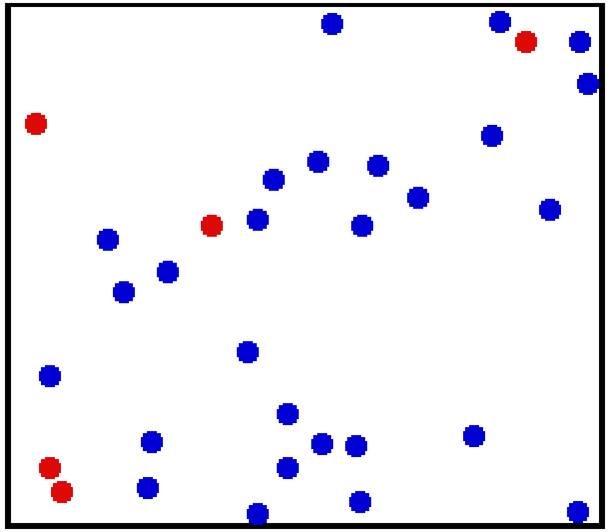
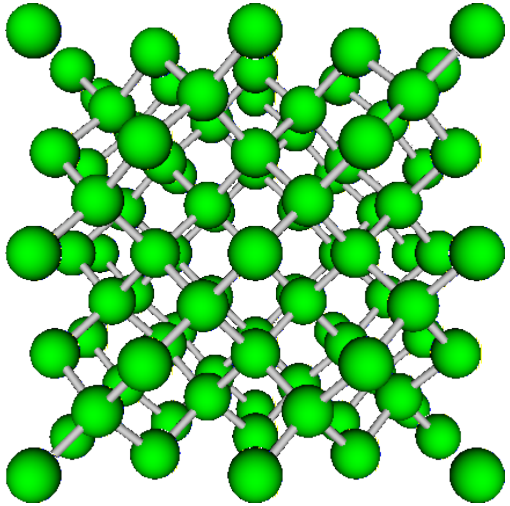
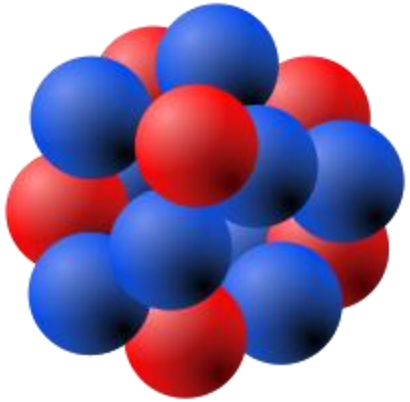
1824.

least partially, for on the one hand the heated air, after having performed its function, having passed round the boiler, goes out through the chimney with a temperature much below that which it had acquired as the effect of combustion; and on the other hand, the water of the condenser, after having liquefied the steam, leaves the machine with a temperature higher than that with which it entered.

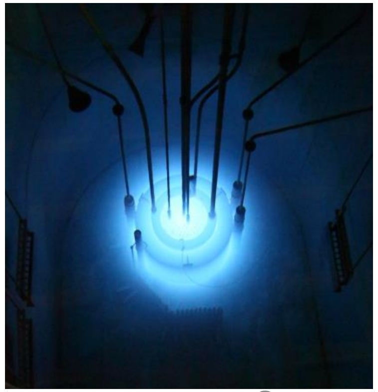
The production of motive power is then due in steam-engines not to an actual consumption of caloric, but *to its transportation from a warm body to a cold body*, that is, to its re-establishment of equilibrium—an equilibrium considered as destroyed by any cause whatever, by chemical action such as combustion, or by any other. We shall see shortly that this principle is applicable to any machine set in motion by heat.

According to this principle, the production of heat alone is not sufficient to give birth to the impelling power: it is necessary that there should also be cold; without it, the heat would be useless. And in fact, if we should find about us only bodies as hot as our furnaces, how can we condense steam? What should we do with it if once produced? We should not presume that we might discharge it into the atmosphere, as is done

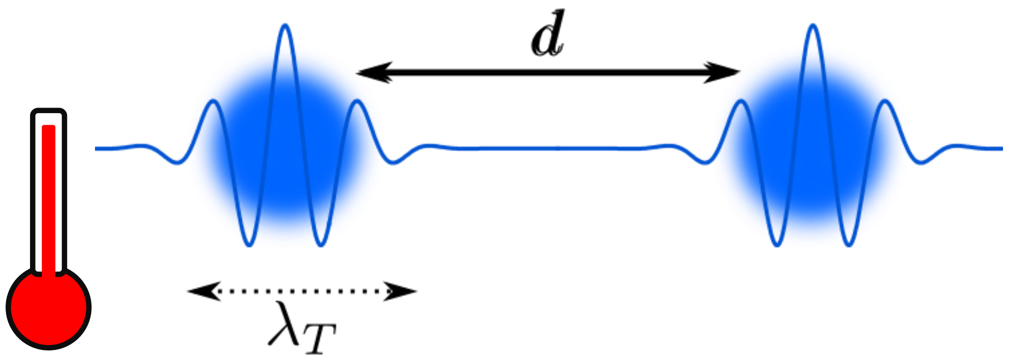
From thermodynamics to statistical physics

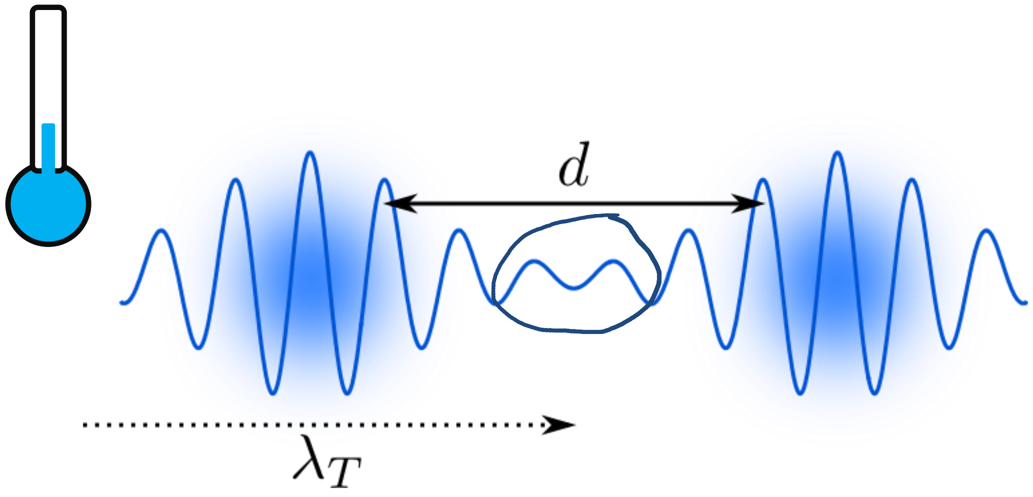




From statistical physics to quantum mechanics



$$d \simeq n^{-1/3} \qquad \lambda_T \simeq \sqrt{\frac{2\pi\hbar^2}{m k_B T}}$$



	Mass	d	T_c
Air	10^{-25} kg	10^{-8} m	10^{-3} K
Material	10^{-30} kg	10^{-10} m	10^{5} K
Nucleus	10^{-27} kg	10^{-15} m	10^{12} K

PHY555 Energy and environment

PHY558B Photovoltaïcs Solar Energy

PHY589 Laboratory course in photovoltaic

PHY563 Material science for energy

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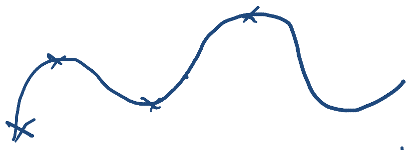
1. Wavefunction

Classical mechanics

Position at all times **r**(t)



Quantum mechanics

Wavefunction $\psi(\boldsymbol{r}, t) \in \mathbb{C}$

$|\psi(\boldsymbol{r}, t)|^2 d^3\boldsymbol{r}$ = *probability to find the particle in a volume* $d^3\boldsymbol{r}$ *around position* ***r*** *at time t.*

$$\langle \mathbf{r}(t) \rangle = \int \mathbf{r} \times |\psi(\mathbf{r}, t)|^2 \, d^3\mathbf{r}$$

$$\langle \mathbf{p}(t) \rangle = -i\hbar \int \psi^*(\mathbf{r}, t) \, \nabla \psi(\mathbf{r}, t) \, d^3\mathbf{r}$$

(not obvious at all !)

2. Operators

Classical mechanics

Position at all times **r**(t)

Quantities

$$\text{Momentum } \boldsymbol{p}(t) = \frac{d\boldsymbol{r}}{dt} \times m$$

$$\text{Energy } E = \frac{p^2}{2m} + V(r)$$

Quantum mechanics

Wavefunction $\psi(\boldsymbol{r}, t) \in \mathbb{C}$

Operators

$$\text{Momentum } \hat{\boldsymbol{p}} = -i\hbar\boldsymbol{\nabla}$$

$$\text{Hamiltonian } \hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{\mathbf{r}}) = -\frac{\hbar^2}{2m}\Delta + V(\hat{\mathbf{r}})$$

$$\hat{p}^2 = -\hbar^2\Delta$$

2. Operators – spectral theorem

Operators have eigenfunctions

$$\hat{O}\Psi = O_n\Psi$$

$$\hat{p}_x \Psi = -i\hbar\partial_x \Psi \stackrel{?}{=} p_x\Psi$$

$$\hookrightarrow \underline{\Psi(x) = \Psi_0 e^{-i\frac{p_x}{\hbar}x}}$$

$$-i\hbar\partial_x\left(\Psi_0 e^{-i\frac{p_x}{\hbar}x}\right) = -i\hbar\Psi_0\left(-\frac{ip_x}{\hbar}e^{-\frac{ip_x}{\hbar}x}\right)$$

$$= p_x\Psi(x)$$

Eigenfunctions form a basis for wavefunctions

$$\hat{O}\Psi = ? = \hat{O}\left(\sum c_n\phi_n\right) \qquad \Psi(x) = \sum c_n\phi_n(x)$$

$\{\phi_n\}$ such that $\hat{O}\phi_n = O_n\phi_n$

$$\int \phi_m^* \phi_n = \delta_{n,m}$$

3. Measurements

Classical mechanics

Position at all times **r**(t)

Quantities

Value of the corresponding quantity

Quantum mechanics

Wavefunction $\psi(\boldsymbol{r}, t) \in \mathbb{C}$

Operators

Single measurement -> one eigen value
Several measurements -> weighted average

$$\psi = \sum c_n \psi_n \text{ with } \hat{O}\psi_n = O_n \psi_n$$

Single measurement: $p(O_n) = |c_n|^2$

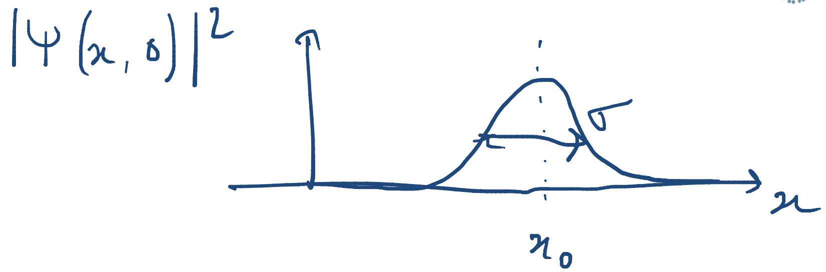
Average value: $\langle \hat{O} \rangle = \sum |c_n|^2 O_n$

4. Time evolution

Classical mechanics	**Quantum mechanics**
Position at all times **r**(t)	Wavefunction $\psi(\boldsymbol{r}, t) \in \mathbb{C}$
Quantities	Operators
Value of the corresponding quantity	Single measurement → one eigen value Several measurements → weighted average
Newton's 2^{nd} law	Schrodinger equation
$$m\frac{d^2\mathbf{r}}{dt^2} = \mathbf{F}$$	$$i\hbar\frac{d\psi}{dt} = \hat{H}\psi$$

4. Time evolution – putting it all together

Initial state $\psi(x,0)$



Schrodinger equation $i\hbar \frac{d\psi}{dt} = \hat{H}\psi$

Spectral theorem $\hat{H}\phi_n = E_n \phi_n$ $\quad \psi = \sum c_n \phi_n$

Calculus 101 $i\hbar \frac{d\phi_n}{dt} = \hat{H}\phi_n = E_n \phi_n \rightarrow \phi_n(t) = \phi_n(0)\, e^{-i\frac{E_n}{\hbar}t}$

Time evolution = dephasing $\psi(x,t) = \sum c_n \phi_n(x,0)\, e^{-i\frac{E_n}{\hbar}t}$

Final state $\psi(x,t)$

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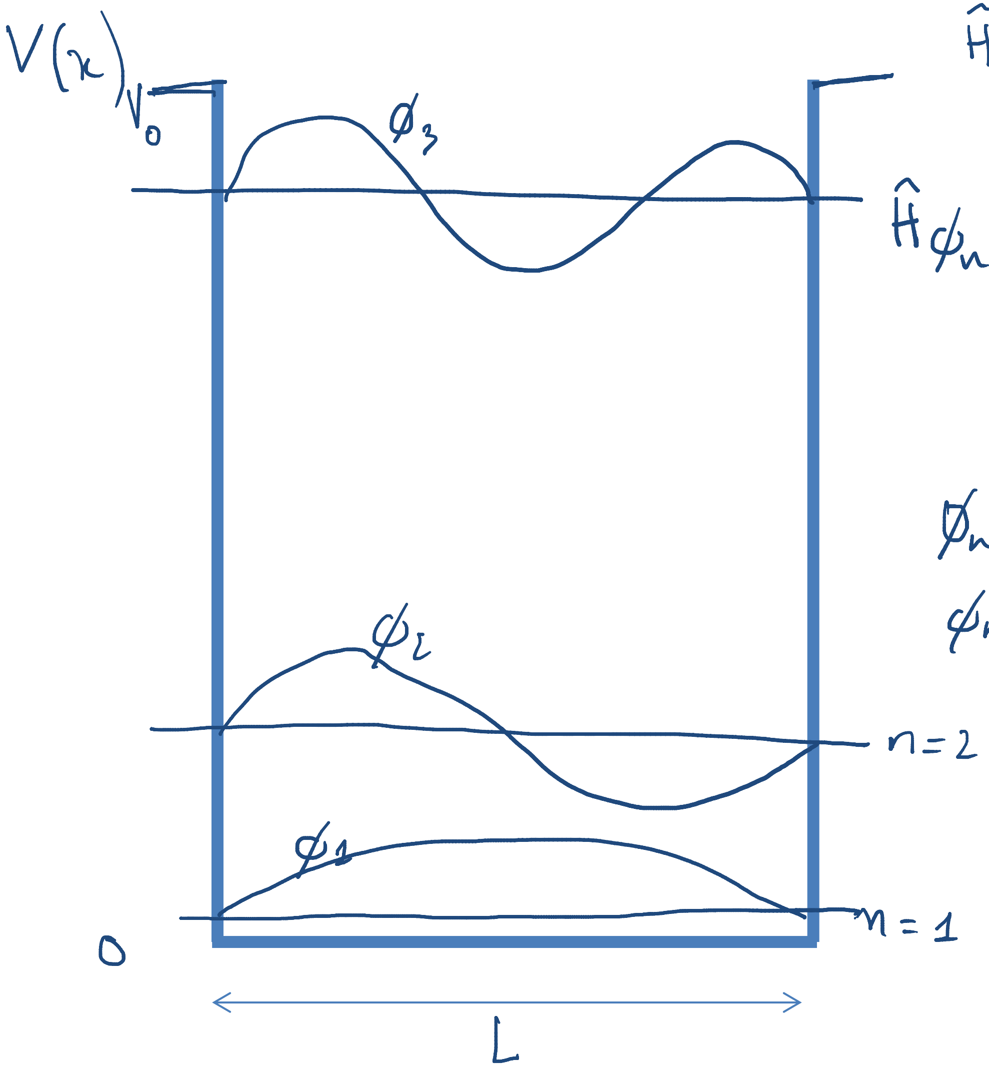
1. Eigen-elements



$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{r}) = -\frac{\hbar^2 \Delta}{2m} + V(r) \qquad 0 \le x \le L \qquad H = -\frac{\hbar^2 \partial_x^2}{2m}$$

$$\dot{f} + \frac{f}{\tau} = 0$$

$$\ddot{f} + \omega_0^2 f = 0$$

$$\hat{H}\phi_n = E_n \phi_n \rightarrow -\frac{\hbar^2}{2m}\partial_x^2 \phi_n = E_n \phi_n \rightarrow \partial_x^2 \phi_n + \frac{2E_n m}{\hbar^2}\phi_n = 0$$

$$\phi_n(x) = A e^{ikx} + B e^{-ikx} \qquad k^2 = \frac{2mE_n}{\hbar^2}$$

$$\phi_n(0) = 0 \qquad A + B = 0 \rightarrow \phi_n = A \times 2i \sin kx$$

$$\phi_n(L) = 0$$

$$\sin kL = 0 \rightarrow kL = n\pi \Rightarrow \text{k such that } k = \frac{n\pi}{L}$$

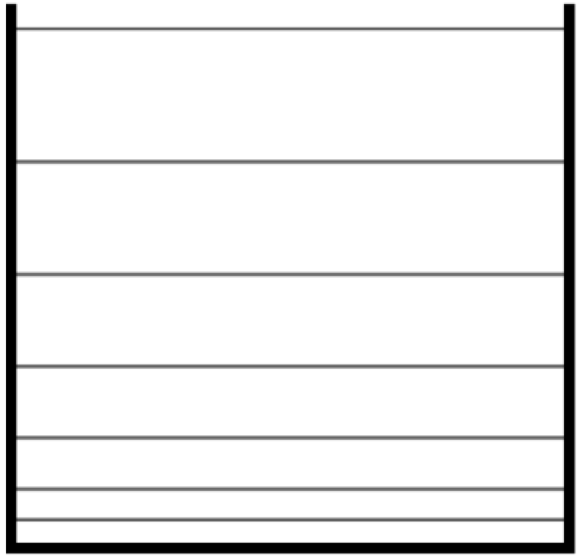
$$E_n = n^2 \times \frac{\pi^2}{L^2}\frac{\hbar^2}{2m}$$

$$\phi_n(x) = A' \sin\left(\frac{n\pi}{L}x\right)$$

$$\int |\phi_n(x)|^2 dx = 1 \rightarrow A' = \sqrt{\frac{2}{L}}$$

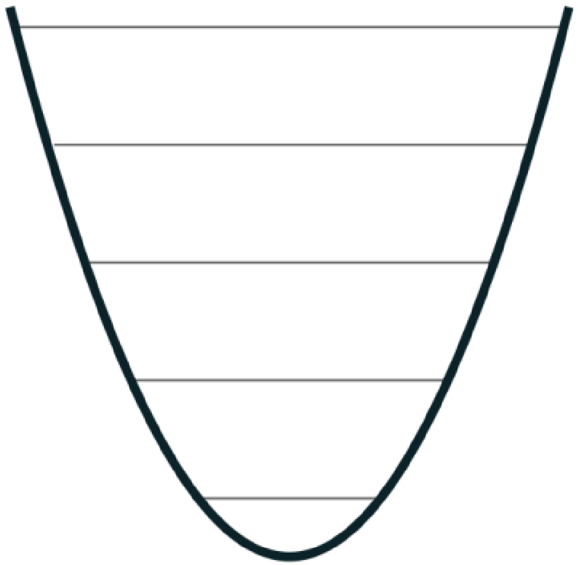
It’s a trap !

Flat well



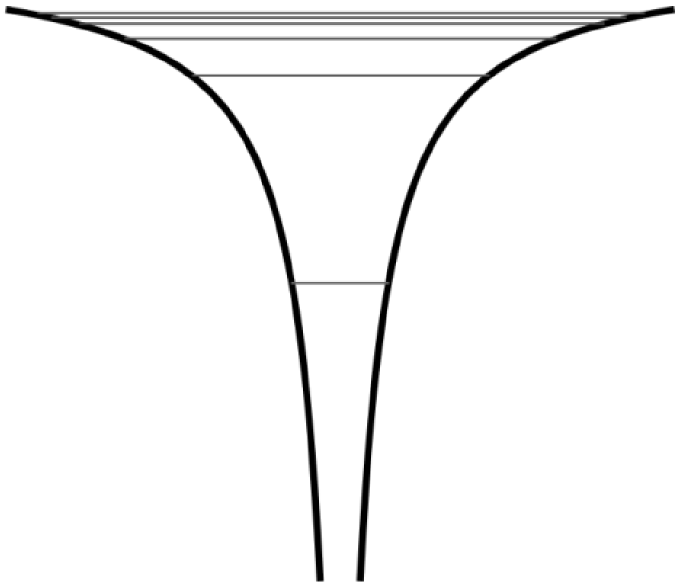
$$E_n = E_0 \times n^2$$

Harmonic trap



$$E_n = E_0 \left(n + \frac{1}{2}\right)$$

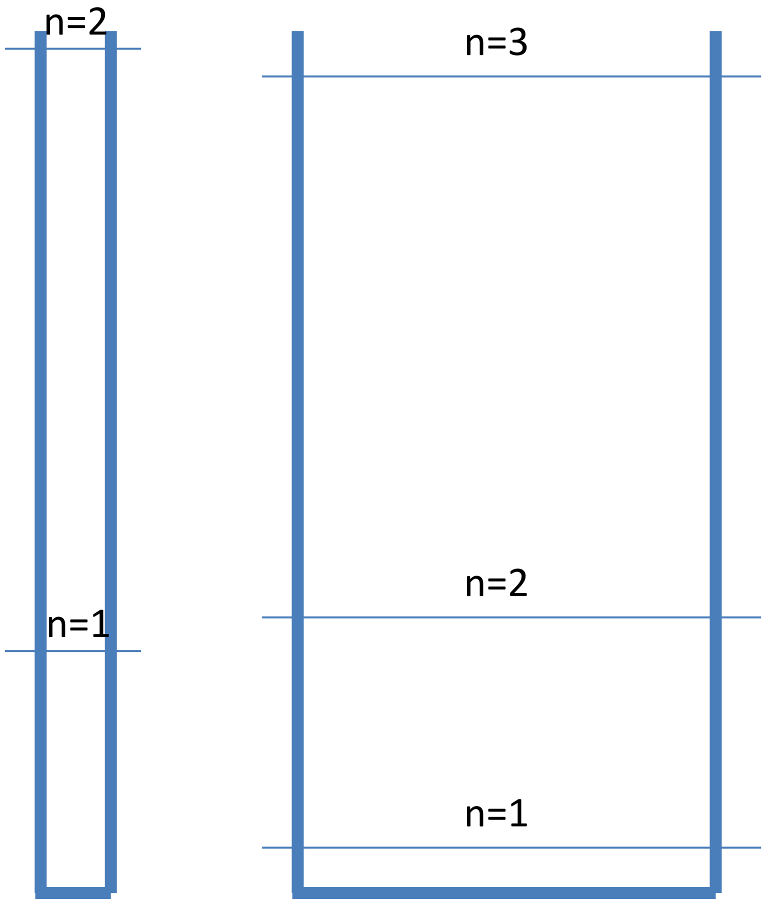
Coulomb potential



$$E_n = -E_0/n^2$$

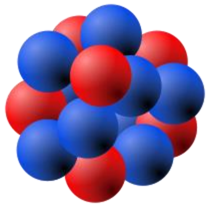
Confinement → discrete energy levels

Application to energy issues



$$E_0 = \frac{\pi^2 \hbar^2}{2mL^2}$$

Nucleus



$m = 10^{-27}$ kg

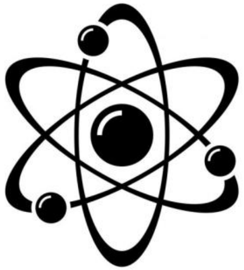
$L = 10^{-15}$ m

$E_0 \simeq \frac{10 \; 10^{-68}}{2 \; 10^{-27} \; 10^{-30}} = 5 \cdot 10^{-12}$ J

$= 5 \times 10^{7}$ eV

50 MeV

Atom



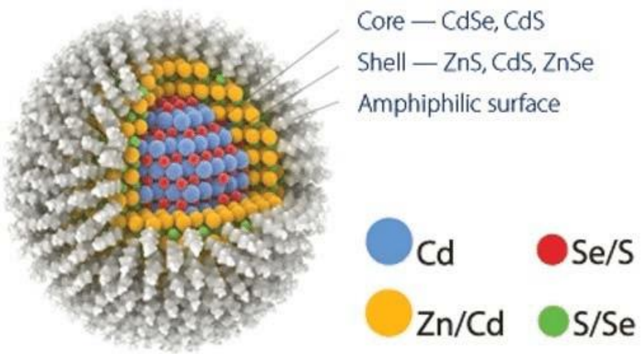
$m = 10^{-30}$ kg

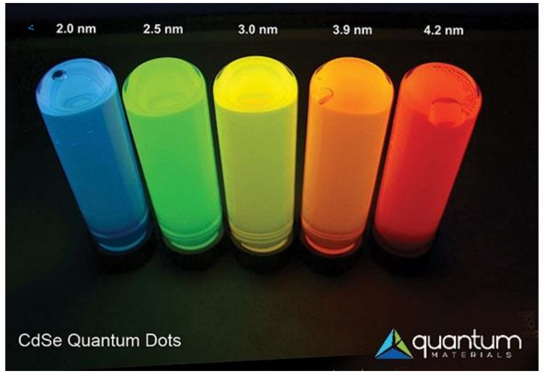
$L = 10^{-10}$ m

$E_0 = \frac{10 \; 10^{-68}}{2 \; 10^{-30} \; 10^{-20}} = 5 \; 10^{-18}$

$= 50$ eV

Quantum dot





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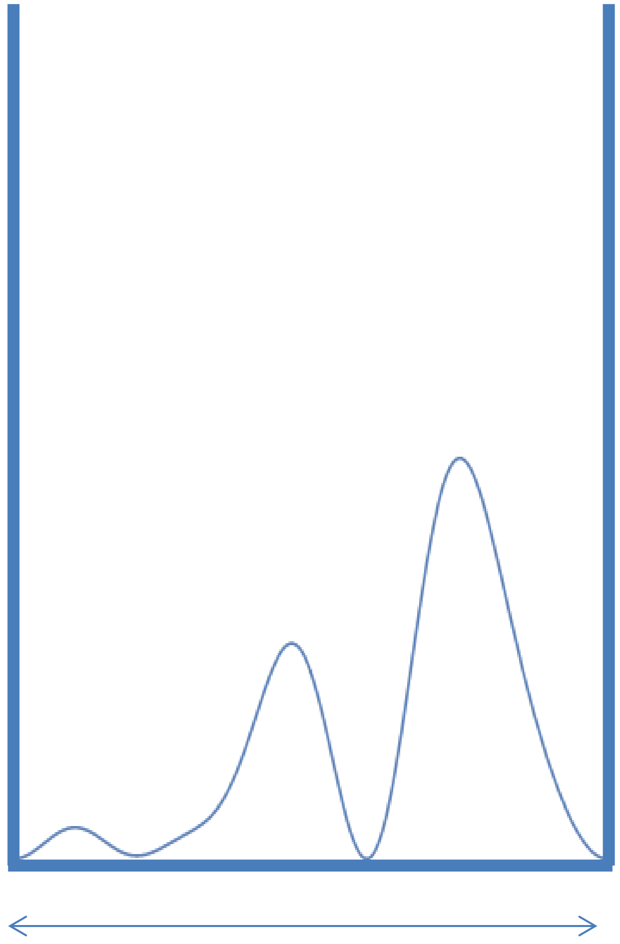
2. Quantum rules (1)



$$|\psi\rangle = \frac{1}{\sqrt{2}}|\phi_2\rangle - \frac{1}{\sqrt{3}}|\phi_3\rangle + \frac{e^{i\pi/4}}{\sqrt{6}}|\phi_5\rangle$$

ϕ_n Hamiltonian eigenstates $\rightarrow \hat{H}\phi_n = E_n \phi_n$ with $E_n = n^2 E_0$

ψ is not an eigenstate : $\hat{H}\psi \neq E\psi$

$\psi = \sum c_n \phi_n$

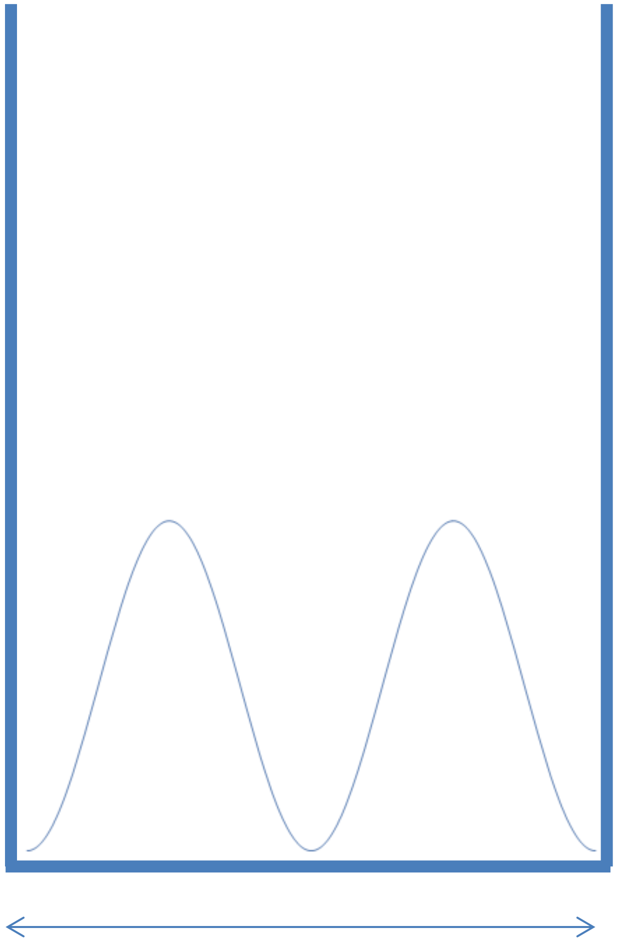
$= \frac{1}{\sqrt{2}} E_2 |\phi_2\rangle - \frac{1}{\sqrt{3}} E_3 |\phi_3\rangle + \frac{e^{i\pi/4}}{\sqrt{6}} E_5 |\phi_5\rangle$

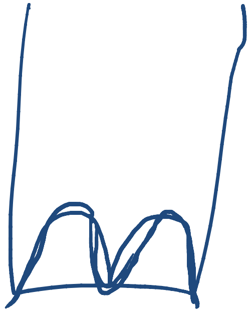
$p(E_0)$	$\rightarrow n=1$	0
$p(2E_0)$	impossible	0
$p(4E_0)$	$\rightarrow n=2$	1/2
$p(9E_0)$	$\rightarrow n=3$	1/3
$p(16E_0)$	$\rightarrow n=4$	0
$p(25E_0)$	$\rightarrow n=5$	1/6

$\langle E \rangle = \frac{1}{2} E_2 + \frac{1}{3} E_3 + \frac{1}{6} E_5$

$= \left[\frac{4}{2} + \frac{9}{3} + \frac{25}{6}\right] E_0 = \frac{55}{6} E_0$

2. Quantum rules (1)





$$|\psi\rangle = |\phi_2\rangle$$

$$\Psi(x) = \sqrt{\frac{2}{L}} \sin \frac{2\pi}{L} x$$

prob. dens. funct: $p(x) = |\Psi(x)|^2 = \frac{2}{L} \sin^2\left[\frac{2\pi}{L} x\right]$

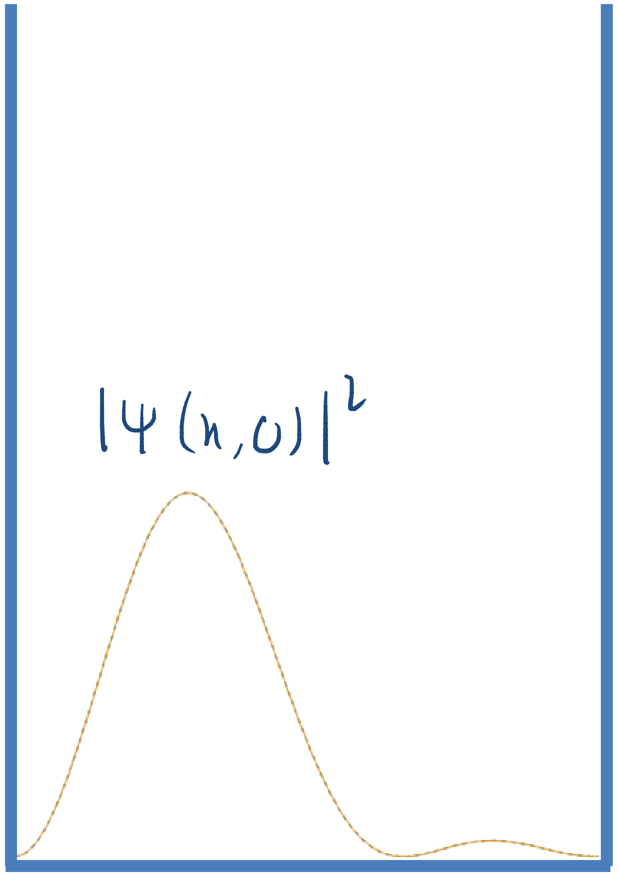
$p(x)\,dx$ = proba. finding the particle @ x up to dx $[x, x+dx]$

average position: $\langle x \rangle = \int dx\, x\, p(x) = \int_0^L dx \left(x \sin^2 \frac{2\pi}{L} x\right) \frac{2}{L} = \frac{L}{2}$

$$|\Psi(t)\rangle = e^{-i\frac{E_2}{\hbar}t} |\phi_2\rangle$$

exactly the same p.d.f as $|\Psi(0,x)|^2$!

2. Quantum rules (2)



$$\psi(x,0) = \sqrt{\frac{1}{L}}\sin\left(\frac{\pi x}{L}\right) + \sqrt{\frac{1}{L}}\sin\left(\frac{2\pi x}{L}\right) = \sum c_n \phi_n$$

$$= \frac{1}{\sqrt{2}}\phi_1(x) + \frac{1}{\sqrt{2}}\phi_2(x)$$

$$\Psi(x,t) = \underbrace{\frac{1}{\sqrt{2}} e^{-\frac{iE_0}{\hbar}t}}_{c_1(t)} \phi_1(x) + \underbrace{\frac{1}{\sqrt{2}} e^{-\frac{i4E_0}{\hbar}t}}_{c_2(t)} \phi_2(x)$$

position

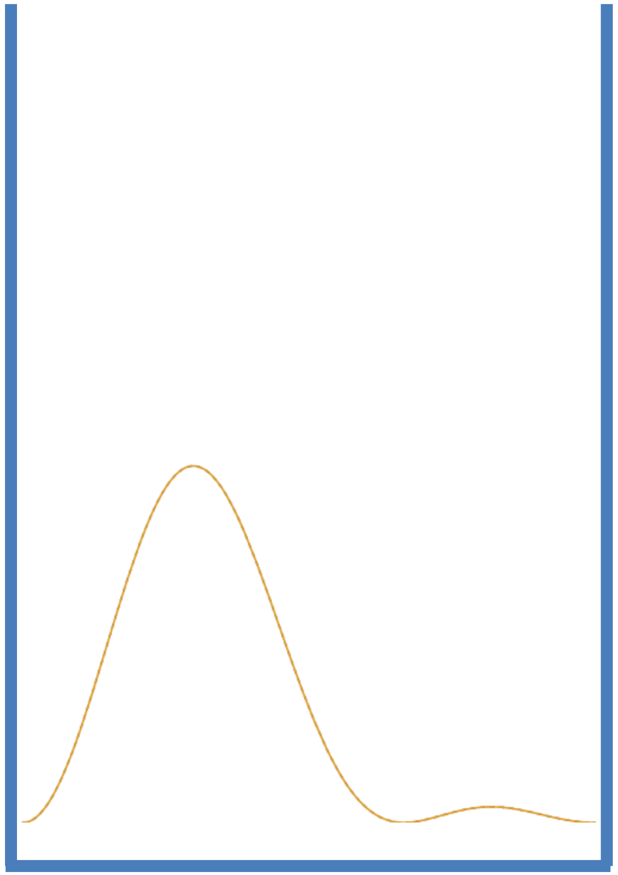
$$\langle x(t)\rangle = \int dx\, x\,|\Psi(x,t)|^2 = \frac{L}{2}\left(1 - \frac{32}{9\pi^2}\cos\left(\frac{3E_0}{\hbar}t\right)\right)$$

Energy

$$\langle E\rangle = p(E_0)\times E_0 + p(4E_0)\times 4E_0$$

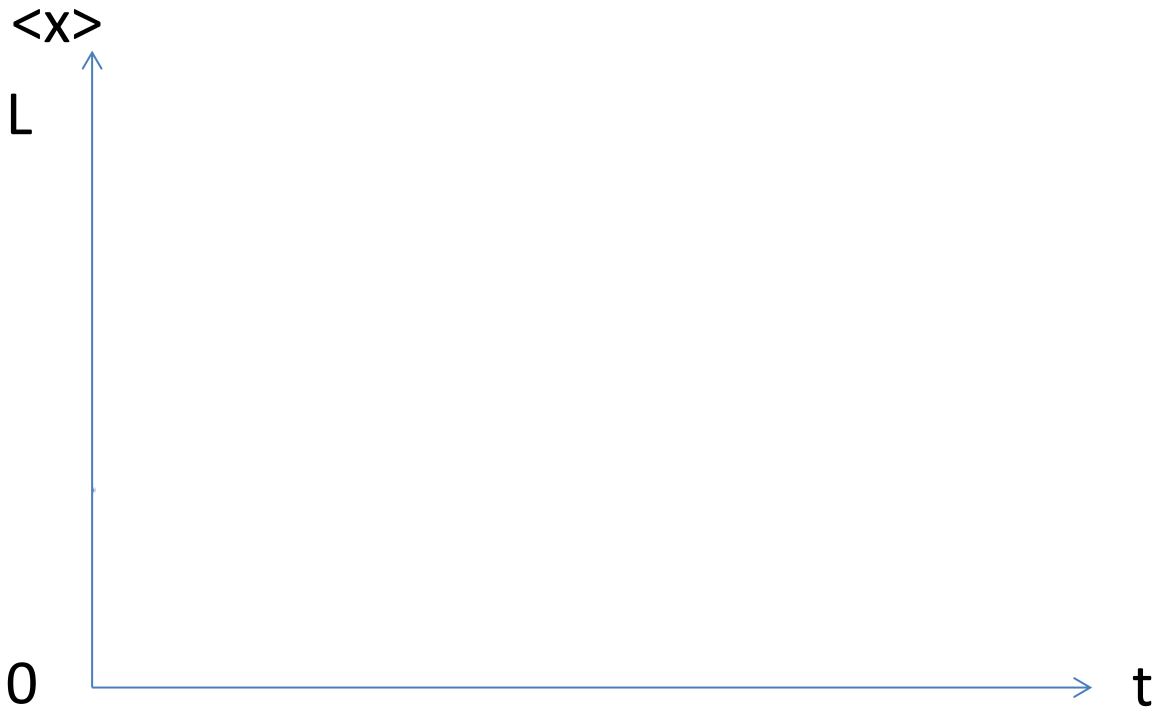
$$= \underbrace{|c_1|^2}_{1/2}\times E_0 + \underbrace{|c_2|^2}_{1/2}\times 4E_0 = \frac{5}{2}E_0 \quad \forall t$$

2. Quantum rules (2)



$$\psi(x,0) = \sqrt{\frac{1}{L}}\sin\left(\frac{\pi x}{L}\right) + \sqrt{\frac{1}{L}}\sin\left(\frac{2\pi x}{L}\right)$$

$$\langle x(t)\rangle = \int x\,|\psi(x,t)|^2\,dx$$



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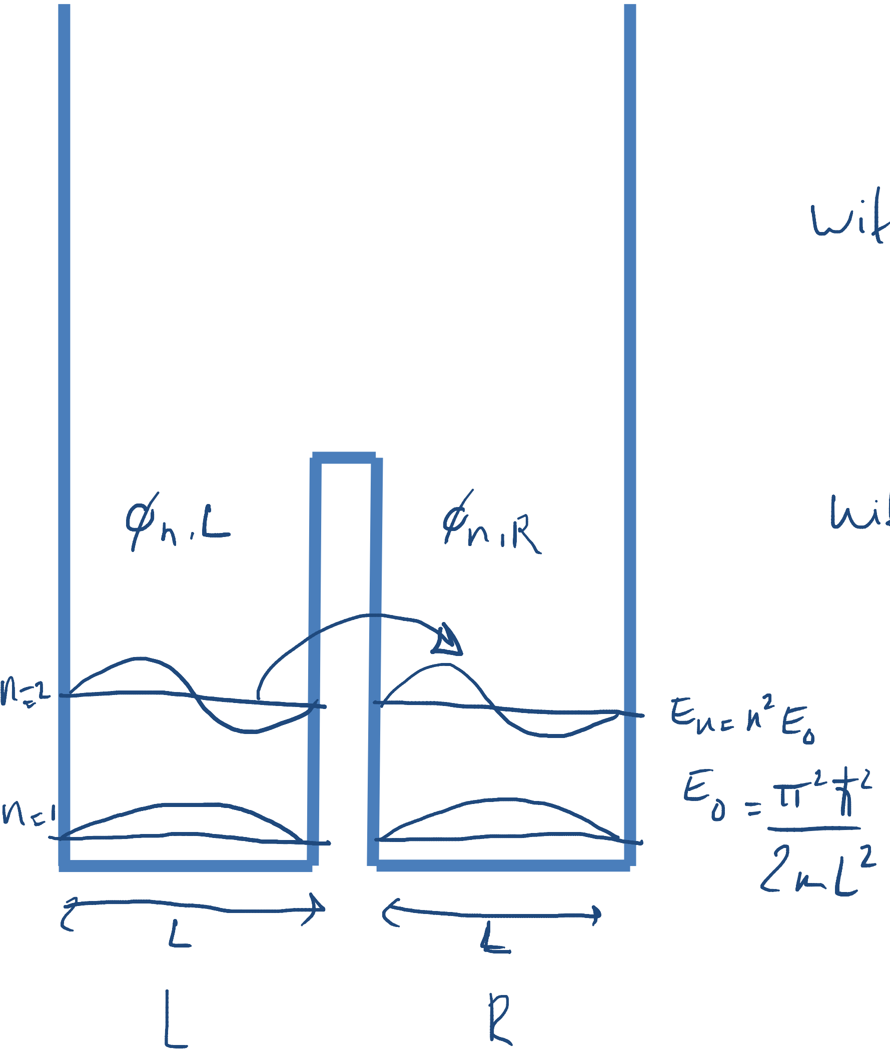
2. Quantum rules (3)



$$\hat{H} = \underbrace{\hat{H}_L + \hat{H}_R}_{\hat{H}_0} + \hat{V}$$

without coupling $\hat{H}_0 |\phi_{n,L}\rangle = E_n |\phi_{n,L}\rangle$

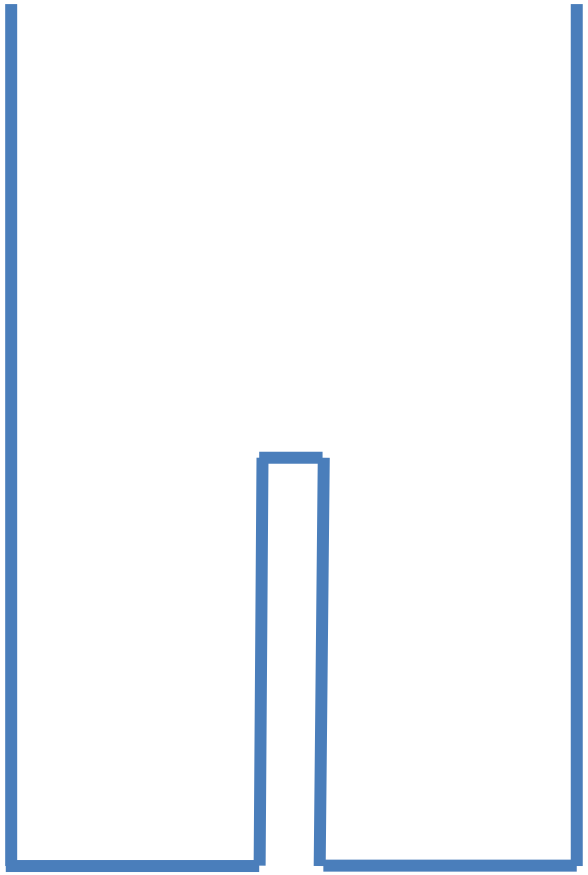
ϕ_n are eigenstate for the Hamiltonian

with coupling $\hat{V} |\phi_{n,R}\rangle = -J |\phi_{n,L}\rangle$ J = strength of coupling

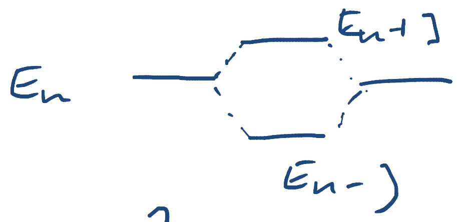
$$\hat{H} |\phi_{n,L}\rangle = E_n |\phi_{n,L}\rangle - J |\phi_{n,R}\rangle \neq E |\phi_{n,L}\rangle$$

$\phi_{n,L}$ are <u>not</u> eigenstates anymore !

2. Quantum rules (3)



$$\hat{H} = \hat{H}_L + \hat{H}_R + \hat{V}$$



$\hat{H}|\phi_{n,L}\rangle = E_n|\phi_{n,L}\rangle - J|\phi_{n,R}\rangle$

$\hat{H}|\phi_{n,R}\rangle = E_n|\phi_{n,R}\rangle - J|\phi_{n,L}\rangle$

$H\phi = E\phi$?

Consider

$|\phi_{n,+}\rangle = \frac{1}{\sqrt{2}}\left(|\phi_{n,R}\rangle + |\phi_{n,L}\rangle\right)$ is a eigenstate with $E_+ = E_n - J$

$\hat{H}|\phi_{n,+}\rangle = \frac{1}{\sqrt{2}}\left[E_n\phi_{nR} - J\phi_{nL} + E_n\phi_{n,L} - J\phi_{nR}\right]$

$= \frac{1}{\sqrt{2}}(E_n - J)(\phi_{nR} + \phi_{nL}) = (E_n - J)|\phi_{n,+}\rangle$

Consider

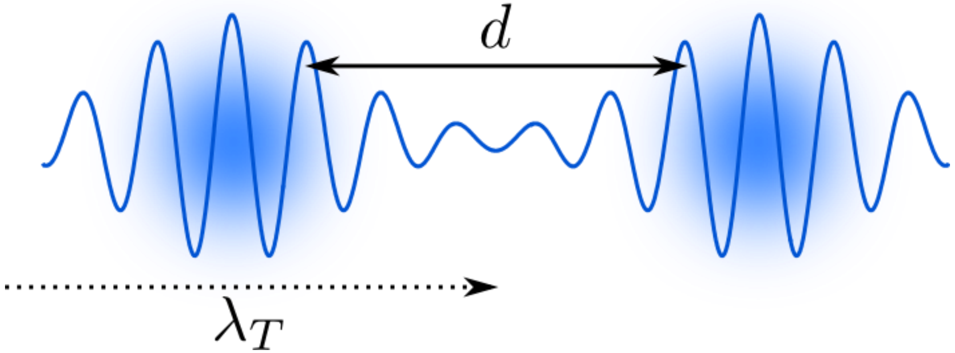
$|\phi_{n,-}\rangle = \frac{1}{\sqrt{2}}\left(|\phi_{n,R}\rangle - |\phi_{n,L}\rangle\right)$ is an eigenstate with $E_- = E_n + J$

$\hat{H}|\phi_{n,-}\rangle = (E_n + J)|\phi_{n,-}\rangle$

STEEM Refresher 1

1. Reminder on thermodynamics
2. Introducing quantum mechanics postulate
3. (Tutorial) Application to the flat potential well – eigen states
4. (Tutorial) Application to the flat potential well – quantum rules
5. (Tutorial) Application to the flat potential well – double well
6. **Conclusion & take home message**

STEEM Refresher 1



Confinement → discrete energy levels

Coupling → lift degeneracy