Week 9

PHY 106 Quantum Physics
Instructor: Sebastian Wüster, IISER Bhopal, 2018

These notes are provided for the students of the class above only.
There is no warranty for correctness, please contact me if you spot a mistake.

3.3) Quantum problems in one dimension

The "particle in a box" already was our first quantum problem in one dimension.

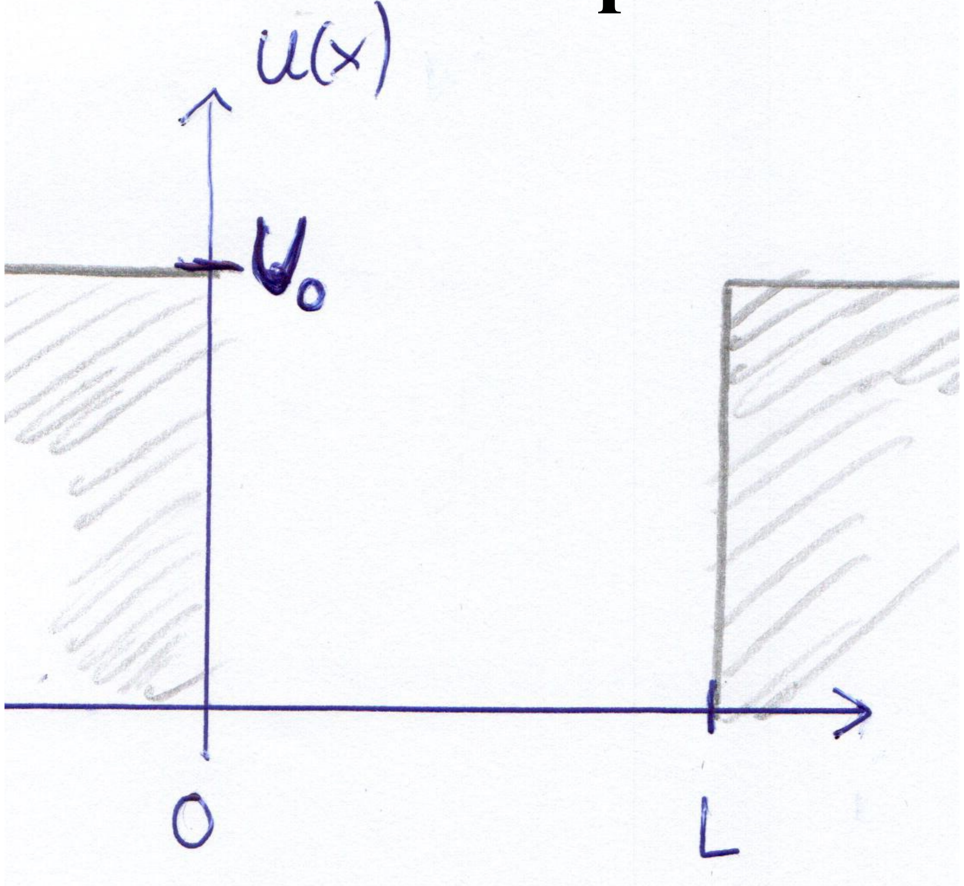
Let us check out some more, which **illustrate** essential concepts of quantum physics and can actually be **solved fully**.

Most more complicated problems can only be solved **approximately** or **numerically** (with a computer).

3.3.1) Particle in Finite box

Of course, and **infinite** energy box *U(x)* does not exist

New realistic **box potential**:



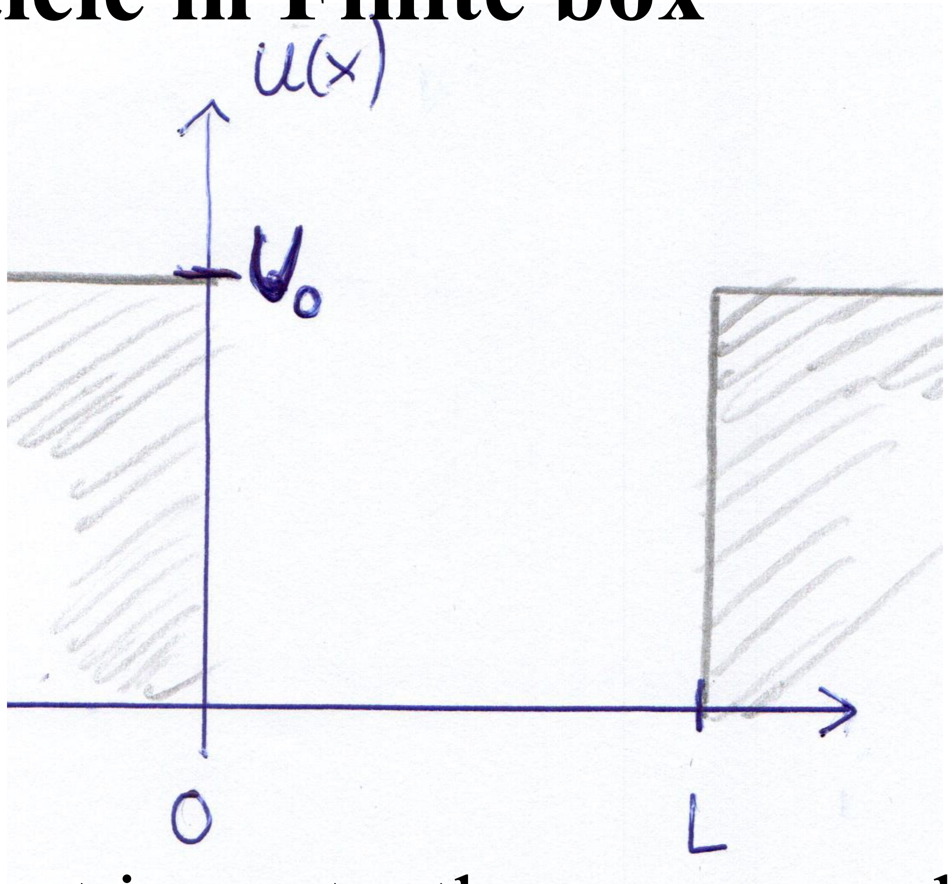
$$U(x) = \begin{cases} 0, & 0 \le x \le L \\ U_0, & \textbf{otherwise} \end{cases} \quad \textbf{(108)}$$

Assume:

$E_n < U_0$

What changes compared to section 3.2.2.1) ???

Particle in Finite box



$$U(x) = \begin{cases} 0, & 0 \le x \le L \\ U_0, & \textbf{otherwise} \end{cases}$$

Most importantly, we can no longer allow the earlier argument why $\phi_n(x) = 0$ outside the box.

For calculation we have to allow $\phi_n(x) \neq 0$ outside

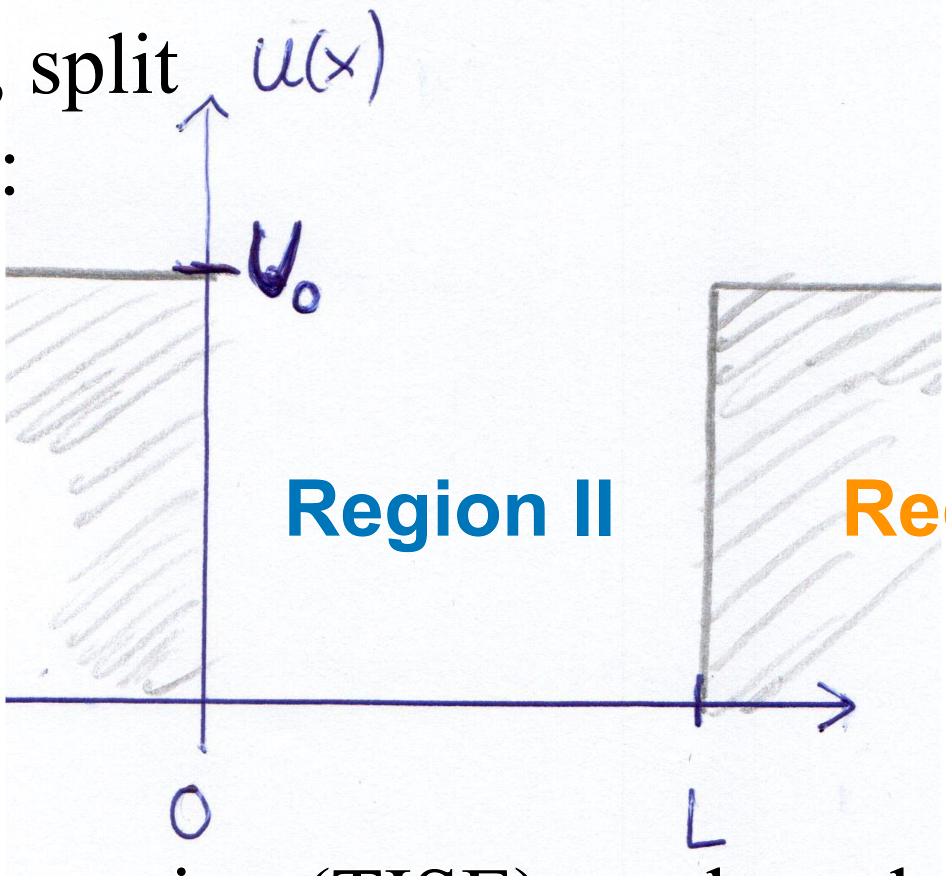
Particle in Finite box

Calculation, split into regions:

$U(x) =$

$0, \ 0 \leq x \leq L$

U_0, **otherwise**



Region I **Region II** **Region III**

Differential equation (TISE) can be solved in each **region**

$$E_n\phi_n(x) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x) \right) \phi_n(x)$$

(I)

$$E_n\phi_n(x) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U_0 \right) \phi_n(x)$$

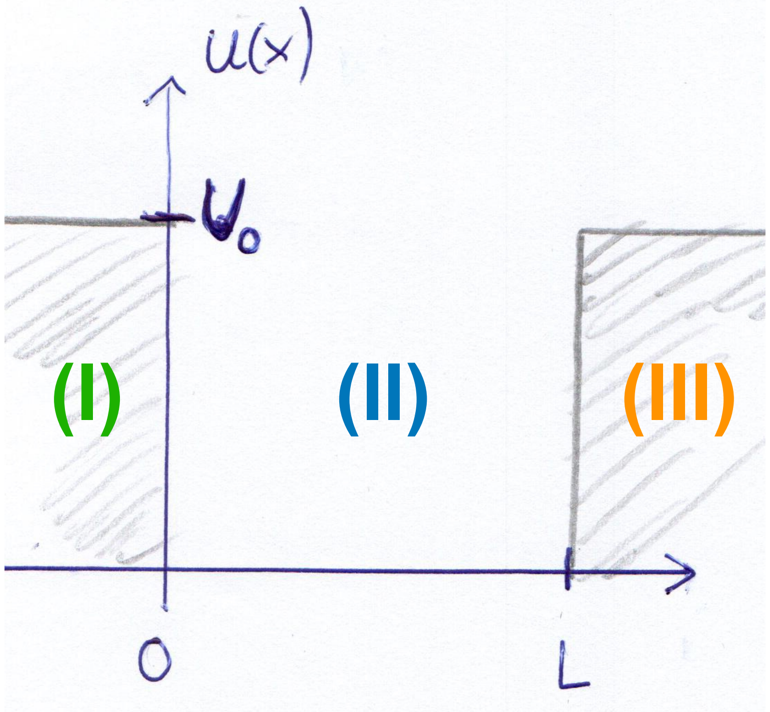
(II)

$$E_n\phi_n(x) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \right) \phi_n(x)$$

(III)

$$E_n\phi_n(x) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U_0 \right) \phi_n(x)$$

Particle in Finite box



Let's look at regions I, III first:

$$E_n\phi_n(x) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U_0\right)\phi_n(x) \quad (109)$$

Rewrite: $$\frac{\partial^2}{\partial x^2}\phi_n(x) - a^2\phi_n(x) = 0$$

(110)

real: $$a = \frac{\sqrt{2m(U_0 - E_n)}}{\hbar}$$

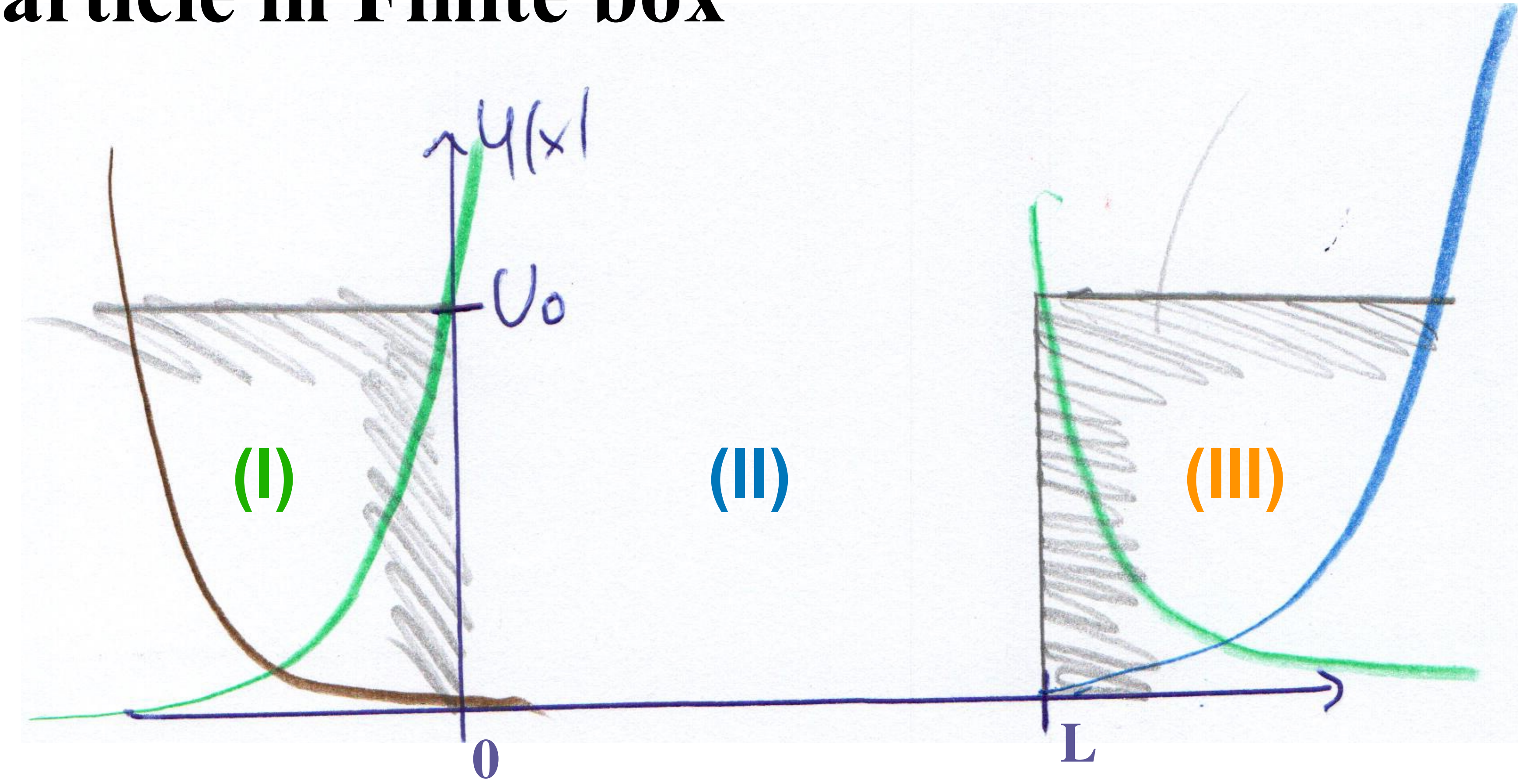
(111)

Solution: In region I: $$\phi_I = Ce^{ax} + De^{-ax}$$

In region III: $$\phi_{III} = Fe^{ax} + Ge^{-ax}$$

[verify by insertion into (110)]

Particle in Finite box



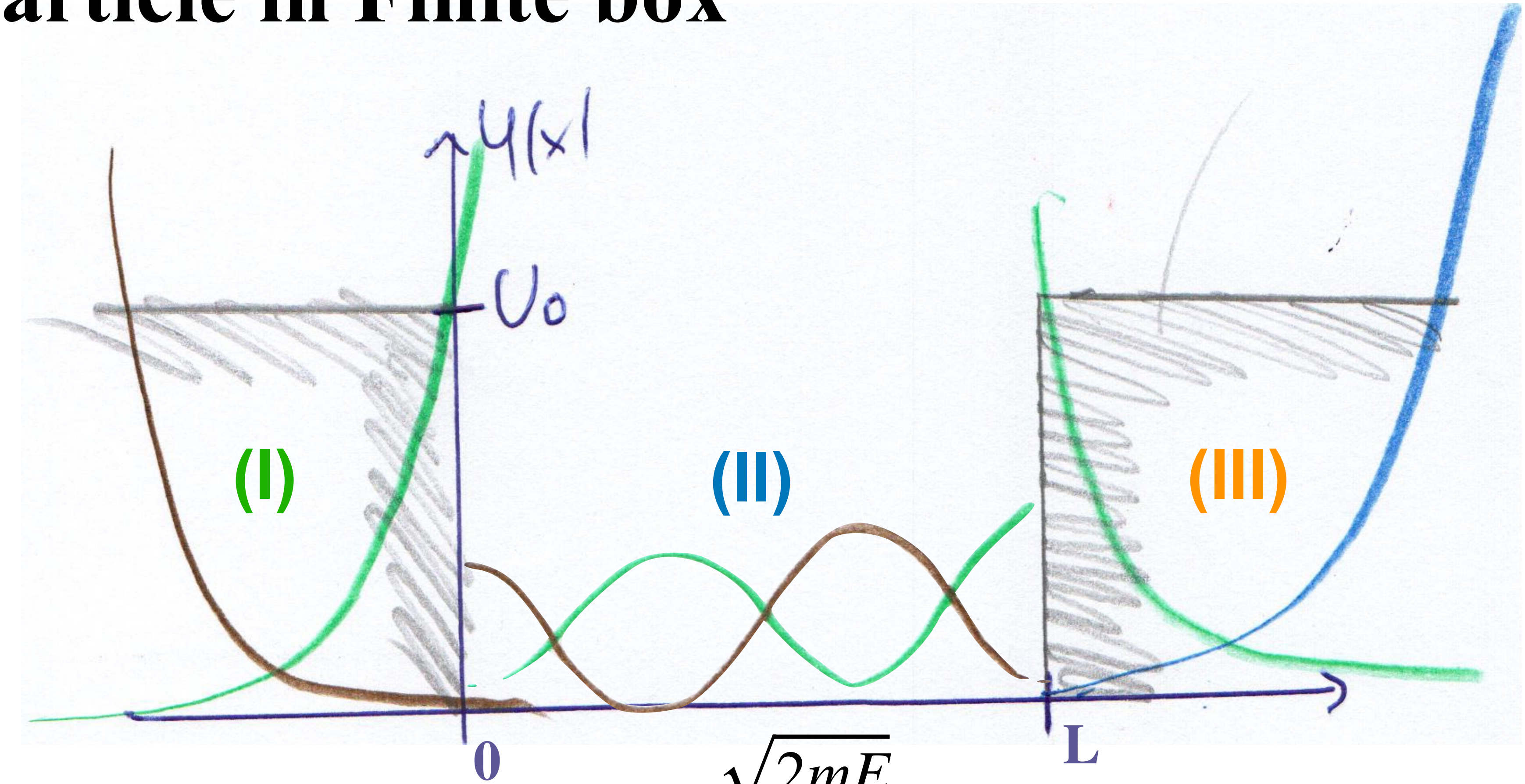
$$\phi_I = Ce^{ax} + De^{-ax}$$

$$\phi_{III} = Fe^{ax} + Ge^{-ax}$$

Need wave function to go to zero at $x \to \pm\infty$

Thus $D=0$, $F=0$

Particle in Finite box



$$k = \frac{\sqrt{2mE}}{\hbar}$$

$$\phi_I = Ce^{ax} \qquad \phi_{III} = Ge^{-ax}$$

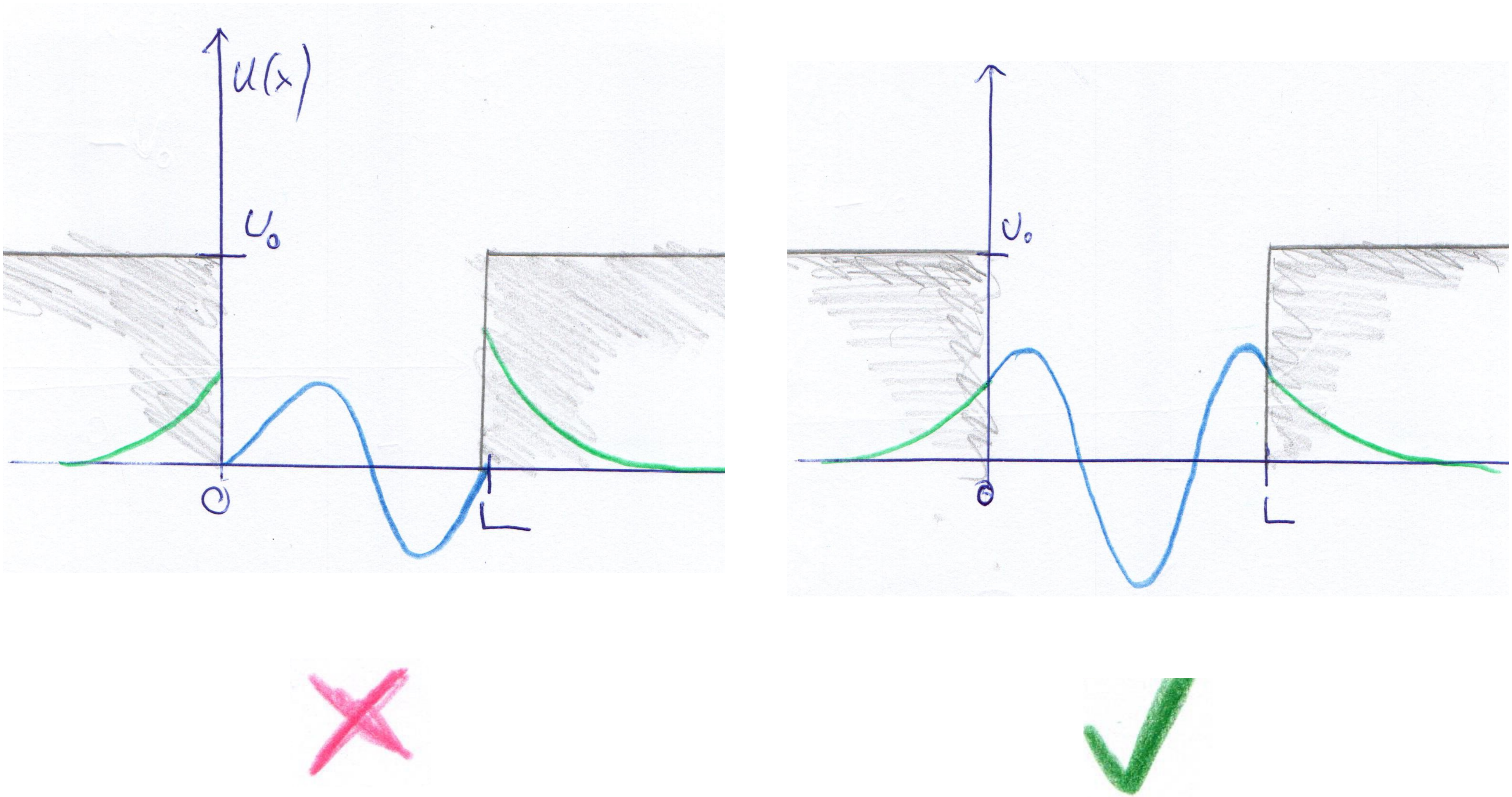
$$\phi_{II} = A\sin\left(kx\right) + B\cos\left(kx\right)$$

Within box, can use Eq. (103) as before.

Finally: $\phi_n(x)$ **and** $\frac{\partial}{\partial x}\phi_n(x)$ have to be continuous at $x=0$ and $x=L$. **(112)**

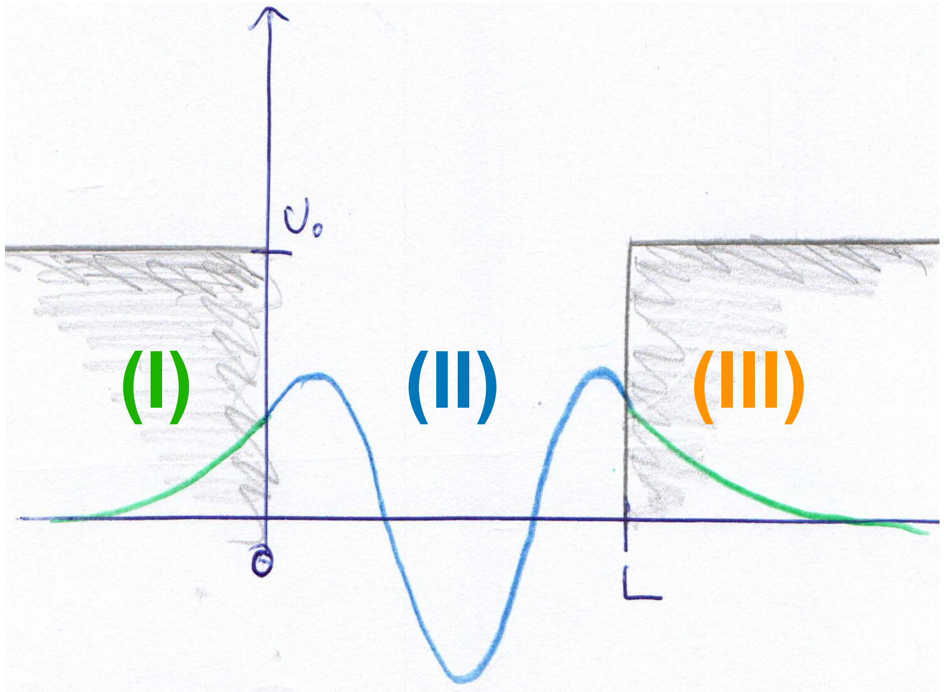
Particle in Finite box

Drawing version of patching together



Particle in Finite box

Math version of patching together



Region I **Region II** **Region III**

$\phi_n(x)$ $\phi_I(0) = \phi_{II}(0)$ $\phi_{II}(L) = \phi_{III}(L)$

Four equations + normalisation =5 equations, only 4 unknowns A,B,C,G

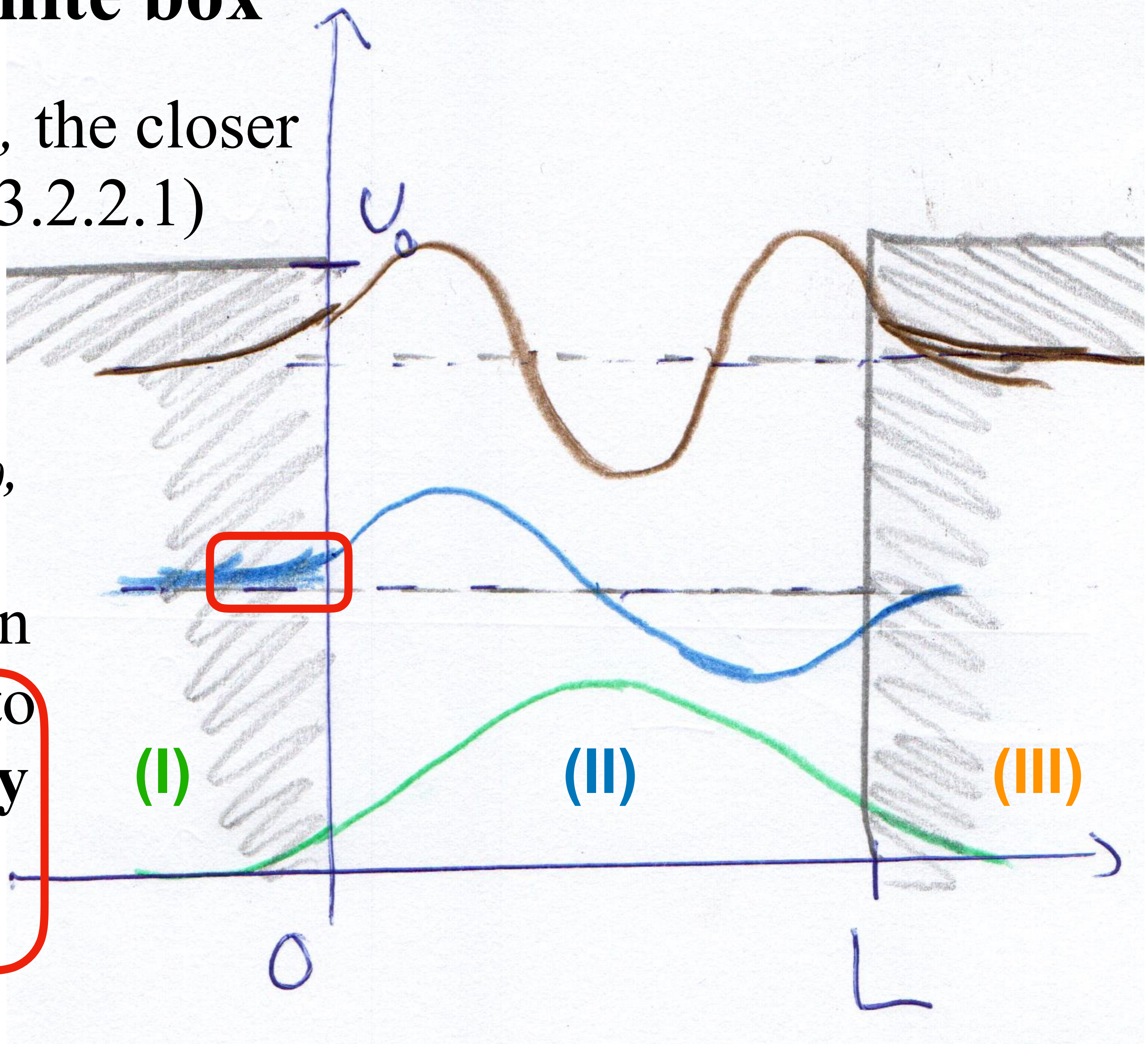
$\frac{\partial}{\partial x}\phi_n(x)$ $\frac{\partial}{\partial x}\phi_I\Big|_{x=0} = \frac{\partial}{\partial x}\phi_{II}\Big|_{x=0}$ $\frac{\partial}{\partial x}\phi_{II}\Big|_{x=L} = \frac{\partial}{\partial x}\phi_{IIi}\Big|_{x=L}$

Only for some k have solution => **quantisation** again

Particle in Finite box

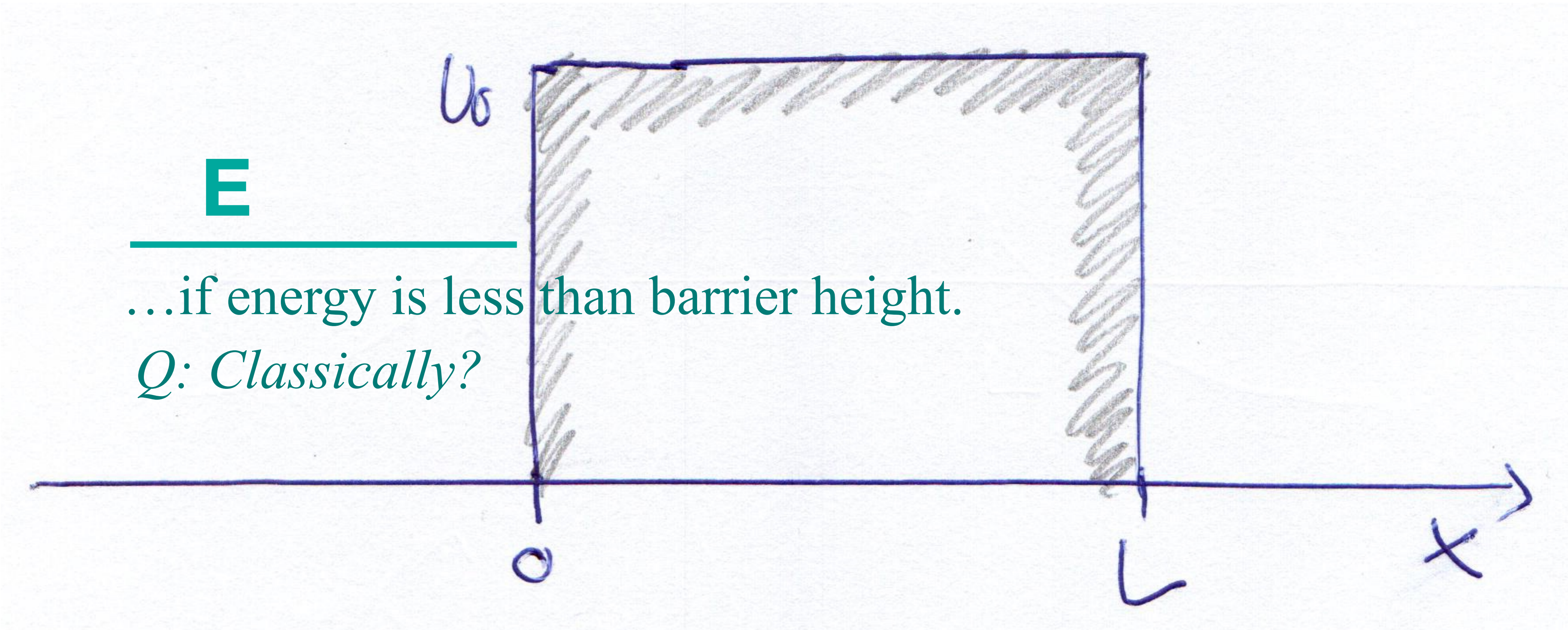
- The higher U_0, the closer it becomes to 3.2.2.1)

- The lower U_0, the more the wave-function penetrates into the **classically forbidden region**



3.3.2) The tunnel effect

We saw that a quantum particle can go where a classical particle can't go….what with a **barrier**?



E

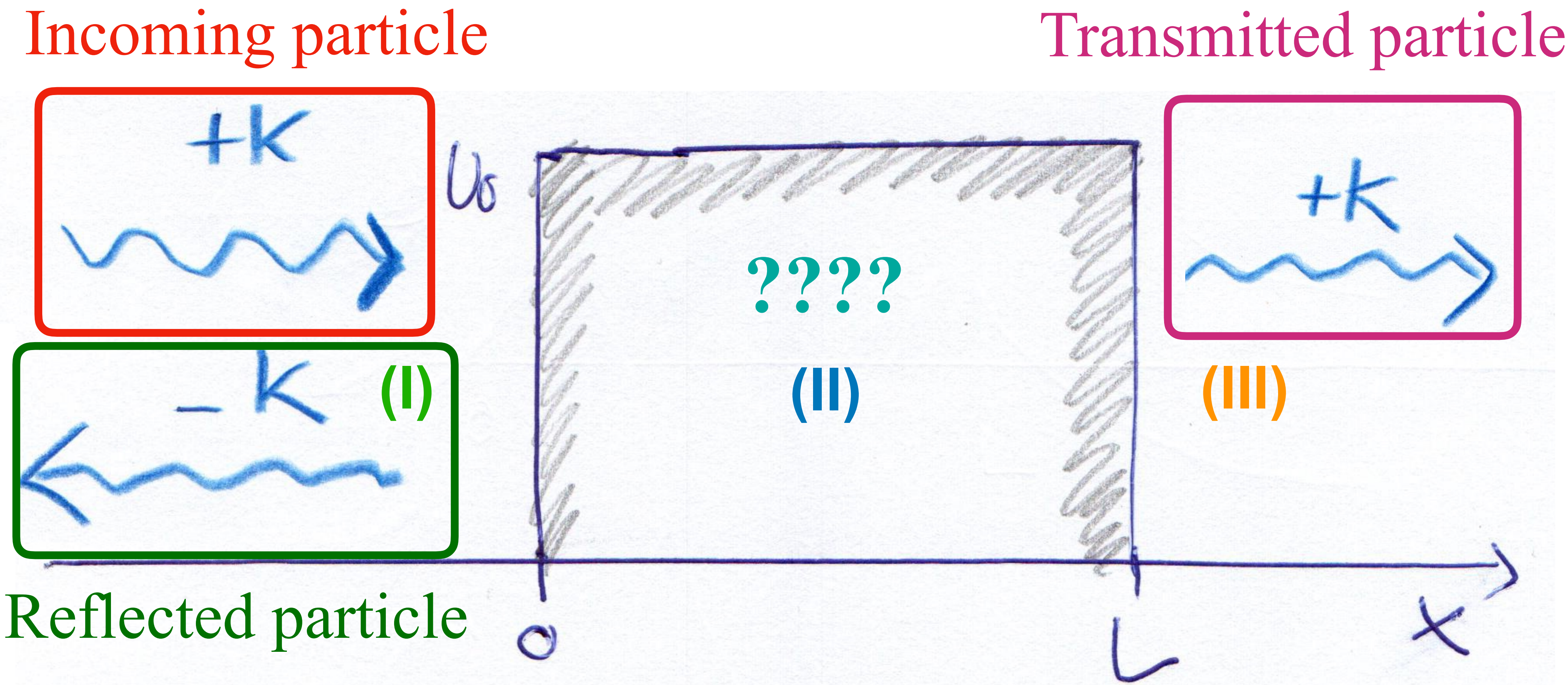
…if energy is less than barrier height.

Q: Classically?

(this is like a flipped finite well)

The tunnel effect

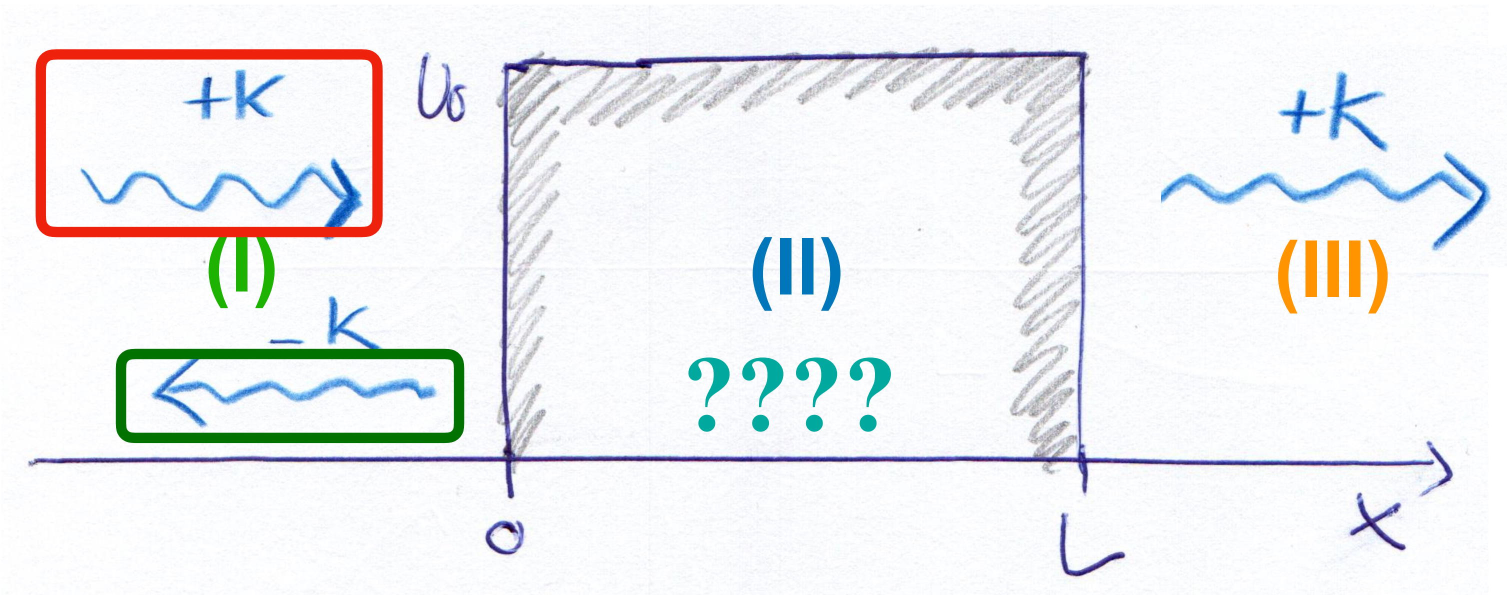
Again can solve TISE in regions



Make an Ansatz based on free particle wave-functions [Eq. (84) , $t=0$]

Above, k symbolizes wave number. +k is a wave moving to the right, -k to the left. Always, the particles has energy E.

The tunnel effect



$$\phi_I = 1 \times \exp(ikx) + \sqrt{R}\exp(-ikx)$$

Inside E<U₀, use earlier results

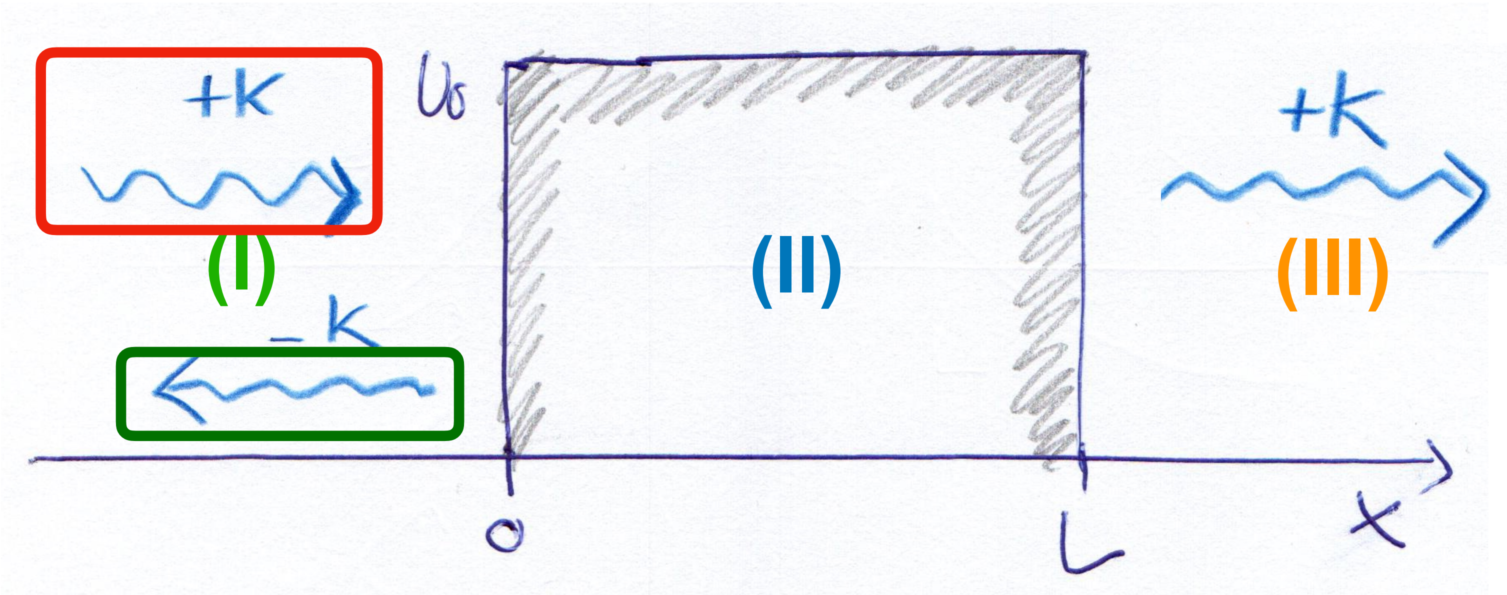
$$\phi_{III} = \sqrt{T}\exp(ikx)$$

T Transmission probability

R Reflection probability

Wavenumber set by energy $k = \frac{\sqrt{2mE_n}}{\hbar}$

The tunnel effect



$$\phi_I = 1 \times \exp(ikx)$$

$$+\sqrt{R}\exp(-ikx)$$

$$\phi_{III} = \sqrt{T}\exp(ikx)$$

$$\phi_{II} = Ae^{ax} + Be^{-ax}$$

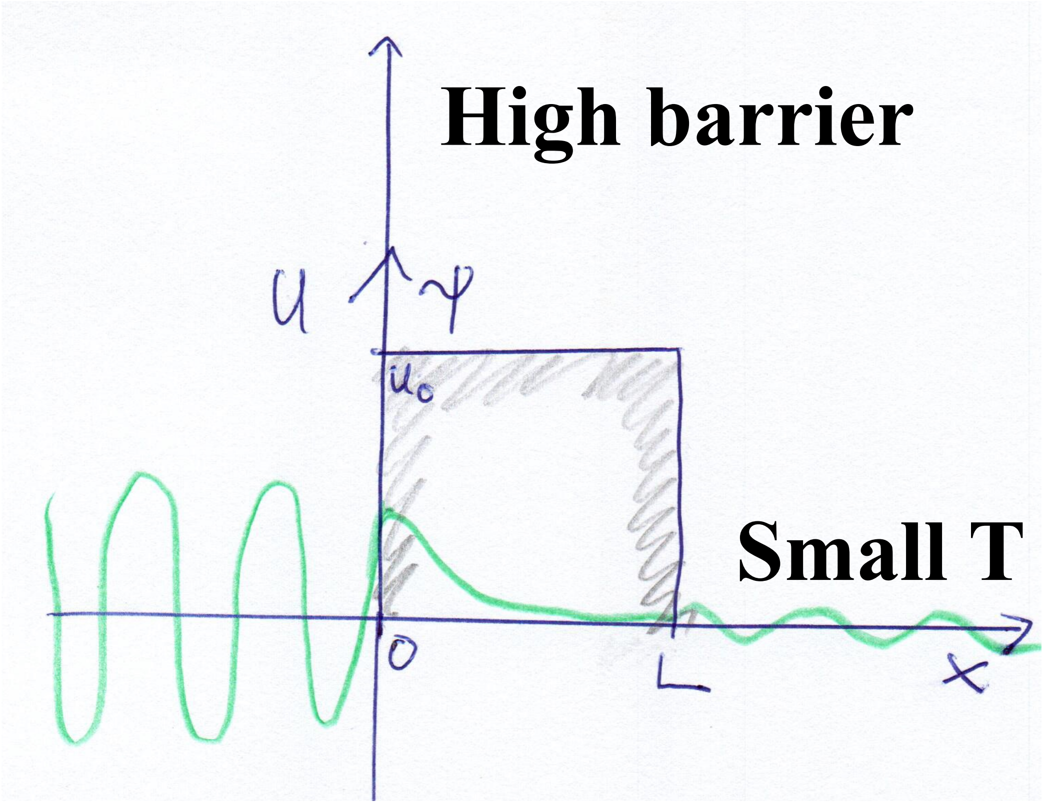
$$a = \frac{\sqrt{2m(U_0 - E_n)}}{\hbar}$$

The tunnel effect

Solution again using continuity

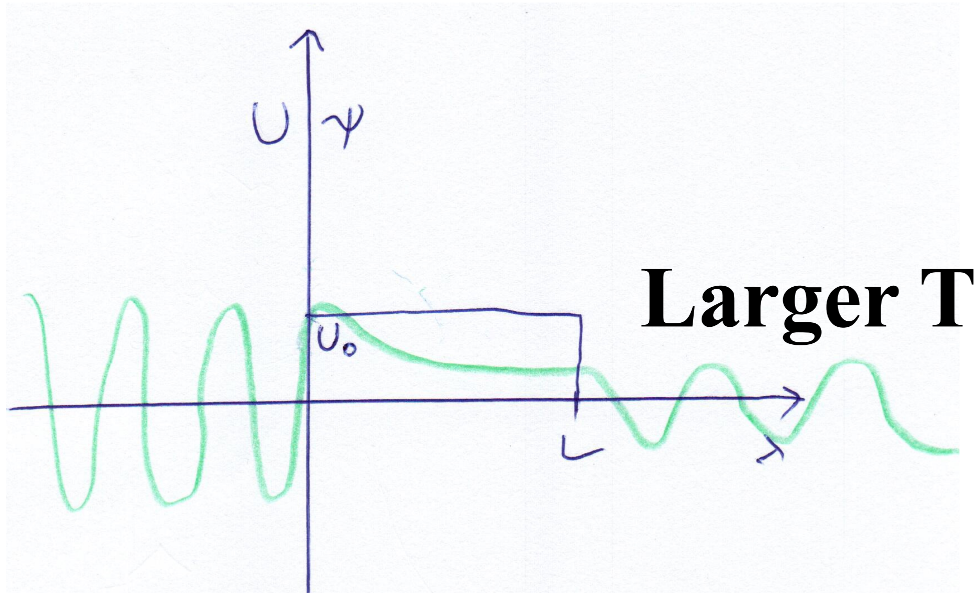
note we draw the real part of Ψ only!!!

High barrier



Small T

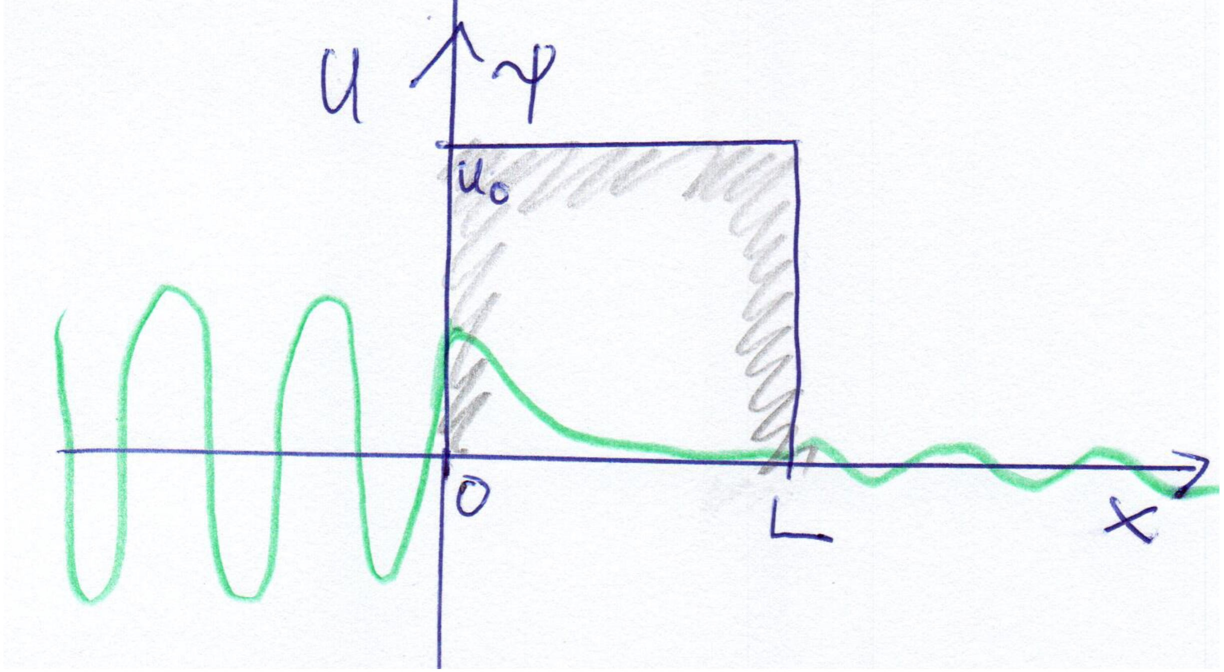
Low barrier



Larger T

Conservation of probability 1 = R+T

The tunnel effect



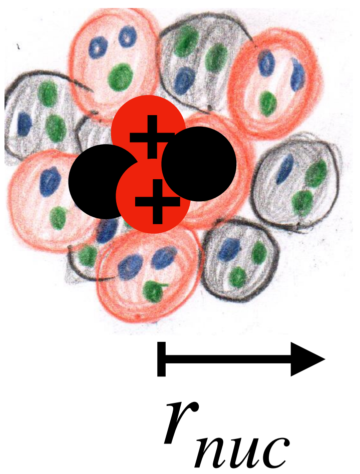
We find **barrier transmission probability**

$$T = e^{-2\kappa L} \qquad \kappa = \frac{\sqrt{2m(U_0 - E)}}{\hbar} \qquad (113)$$

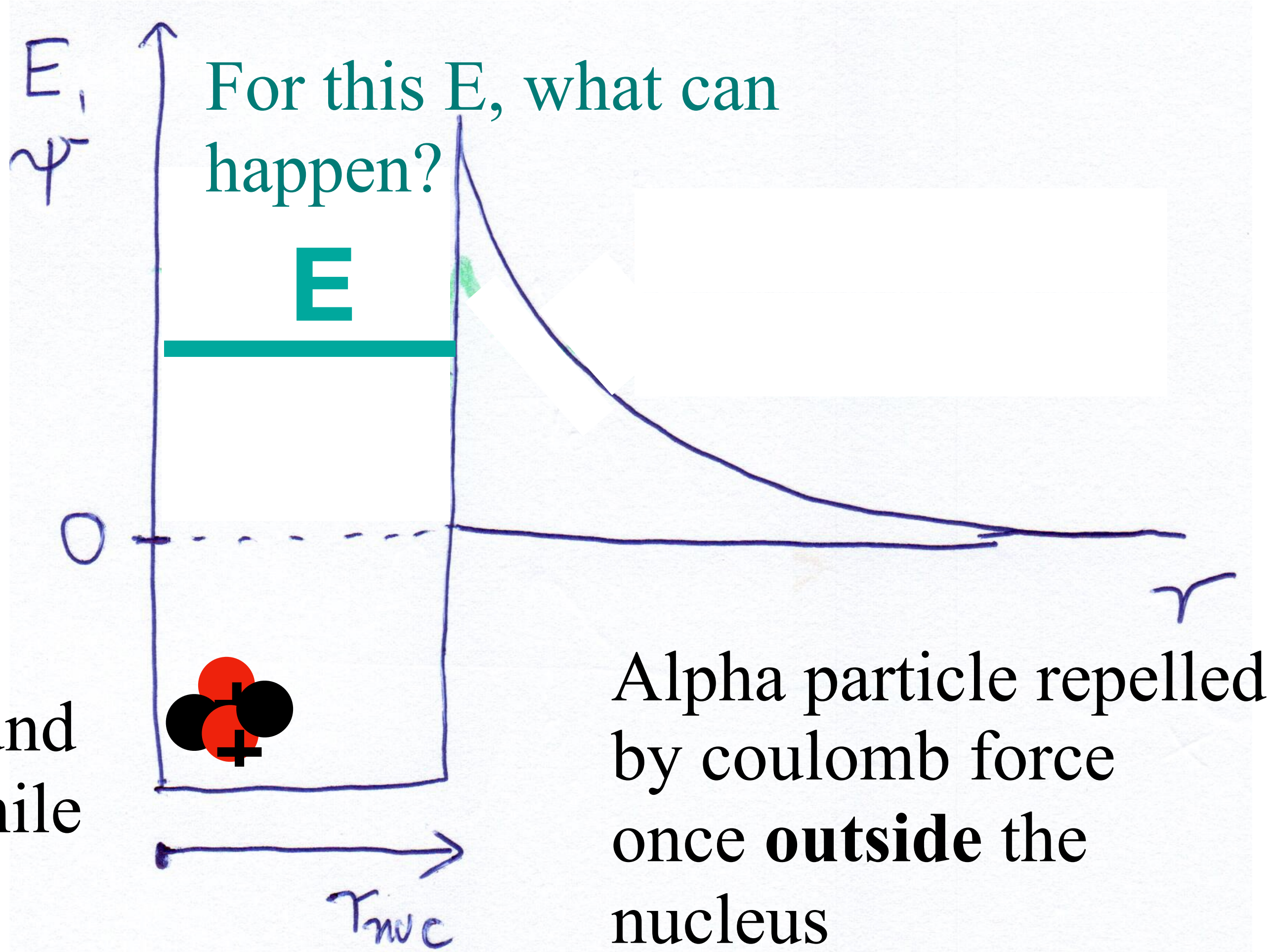
- In principle always nonzero: quantum particle can **“tunnel”** through the barrier.
- In practice exponential dependence on barrier depth L and strength U: only big if $\kappa L \sim 1$

Example I: Nuclear alpha decay

- Tunnel effect only important for microscopic objects.
- Consider atomic-nucleus (3.1.4). A fragment of that can be viewed as an alpha-particle.



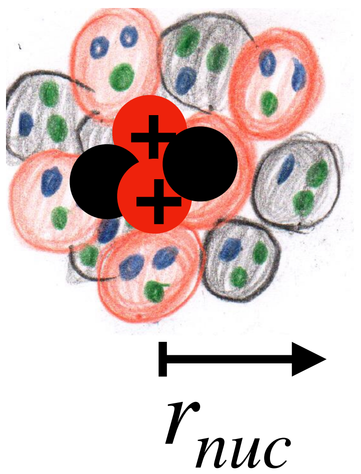
Alpha particle bound by strong force while **inside** the nucleus

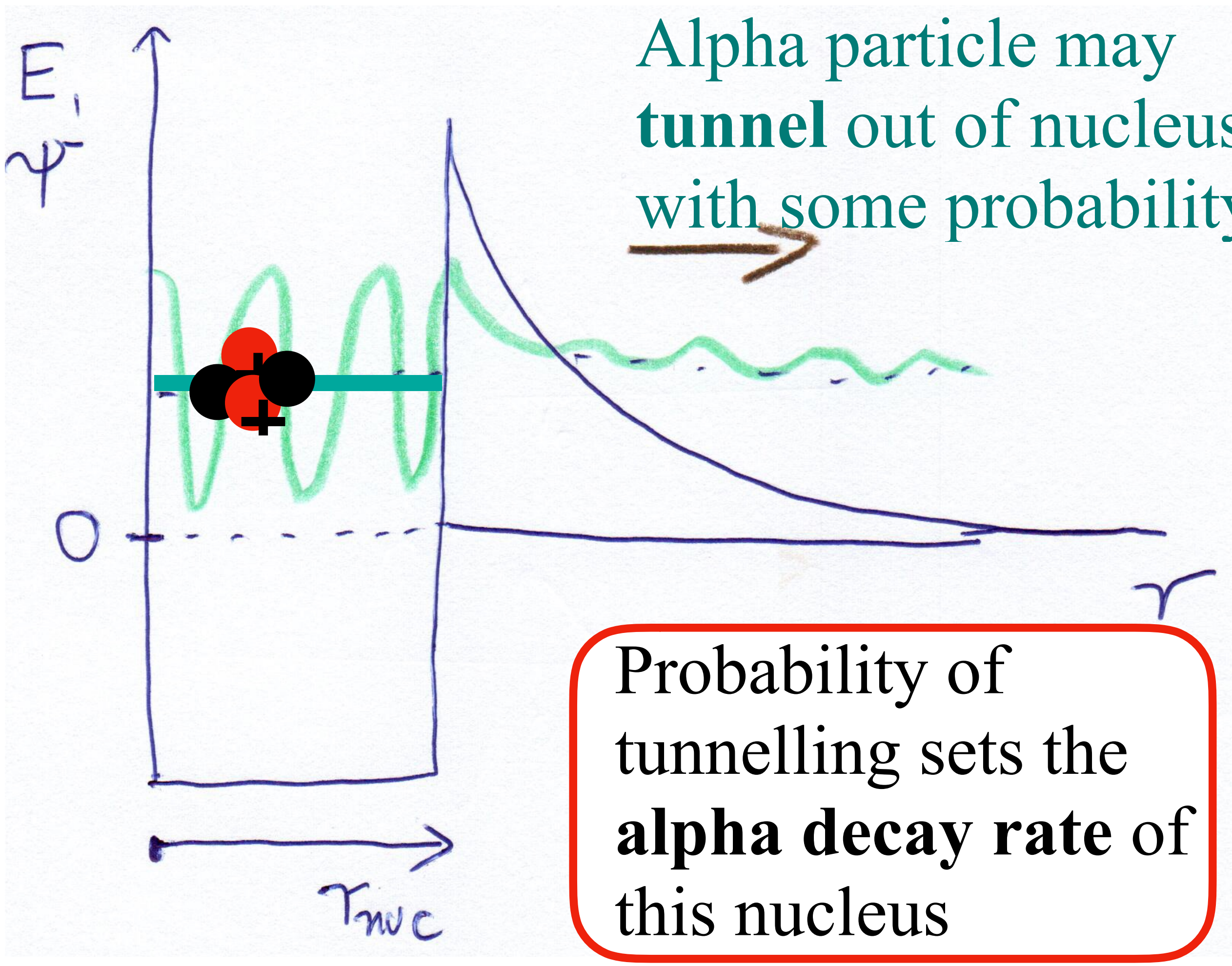


Alpha particle repelled by coulomb force once **outside** the nucleus

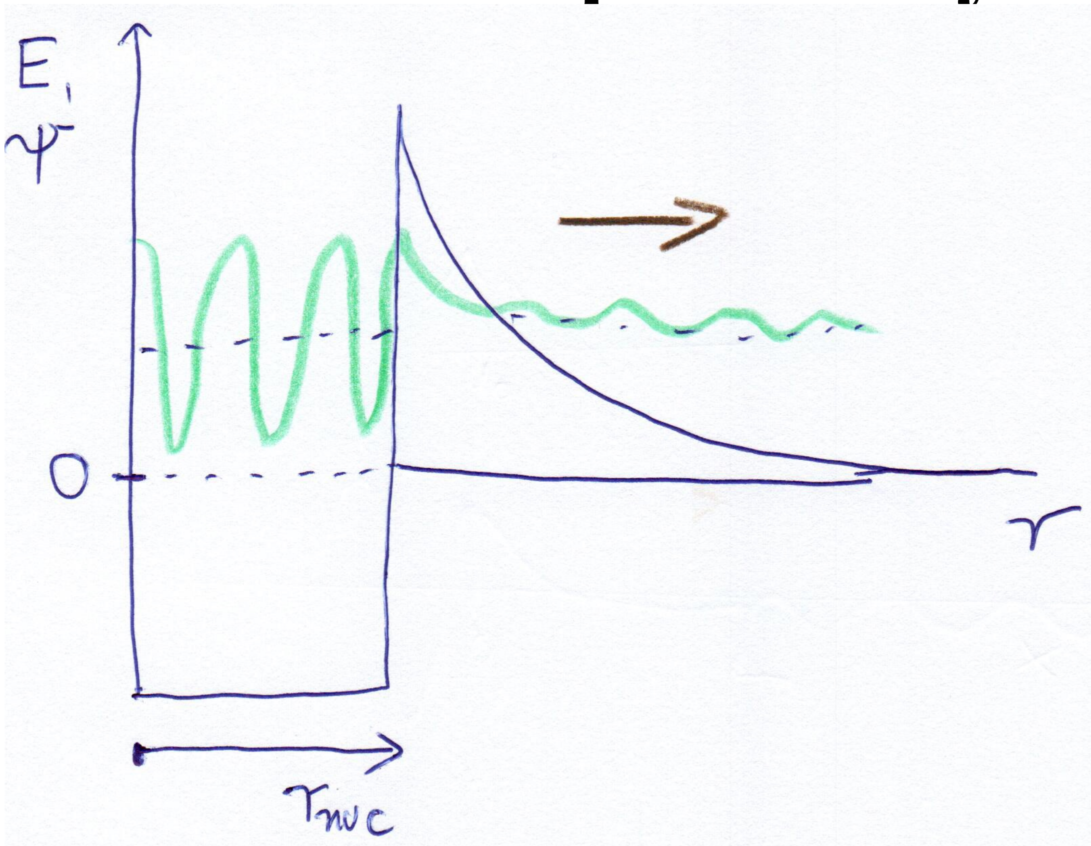
Example I: Nuclear alpha decay

- Tunnel effect only important for microscopic objects.
- Consider atomic-nucleus (3.1.4). A fragment of that can be viewed as an alpha-particle.





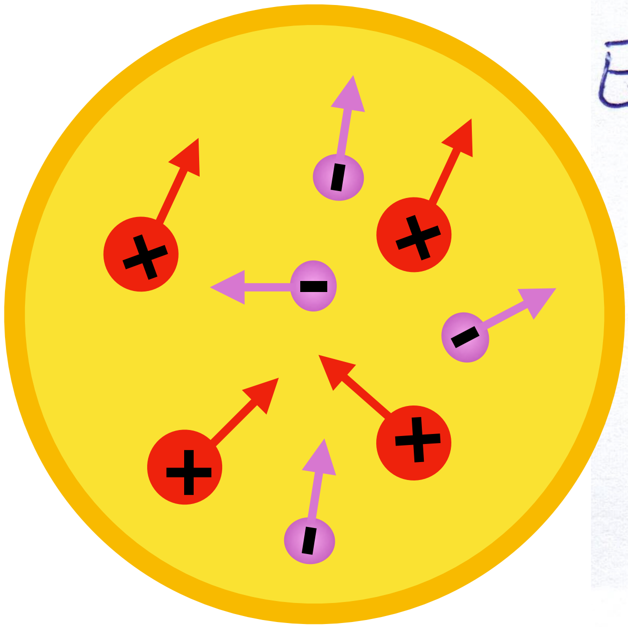
Example I: Nuclear alpha decay

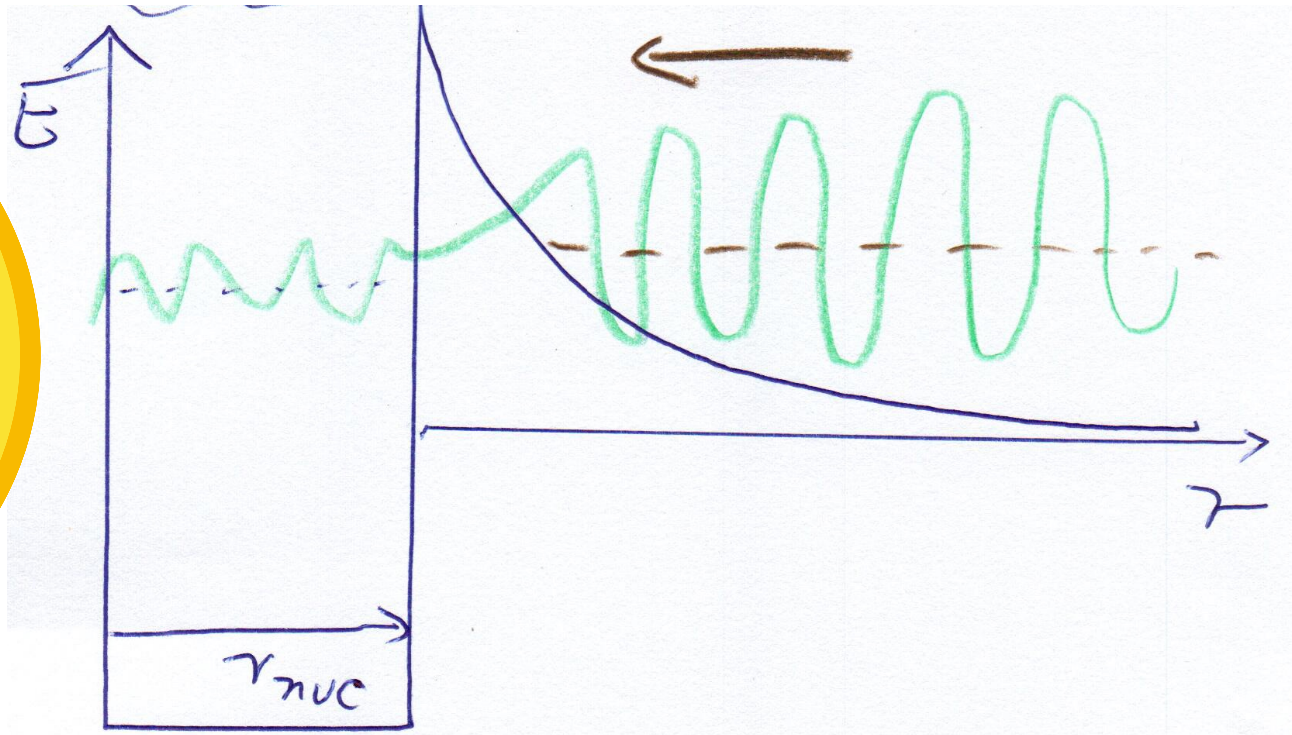


- Tunneling probability can be very low.
- E.g., alpha-decay of ^{238}U nucleus, has a half-life due to alpha decay of $\tau = 4.5 \times 10^9$ years!
- See Eq. (113): Exponential dependence on E and L.

Example II: Nuclear fusion in the sun

- Tunnelling is also crucial in the inverse process.
- How does a proton get **into** the strong force well?
- In solar nuclear fusion: p+p ➜ pp (➜ pn + e^+ + ν)



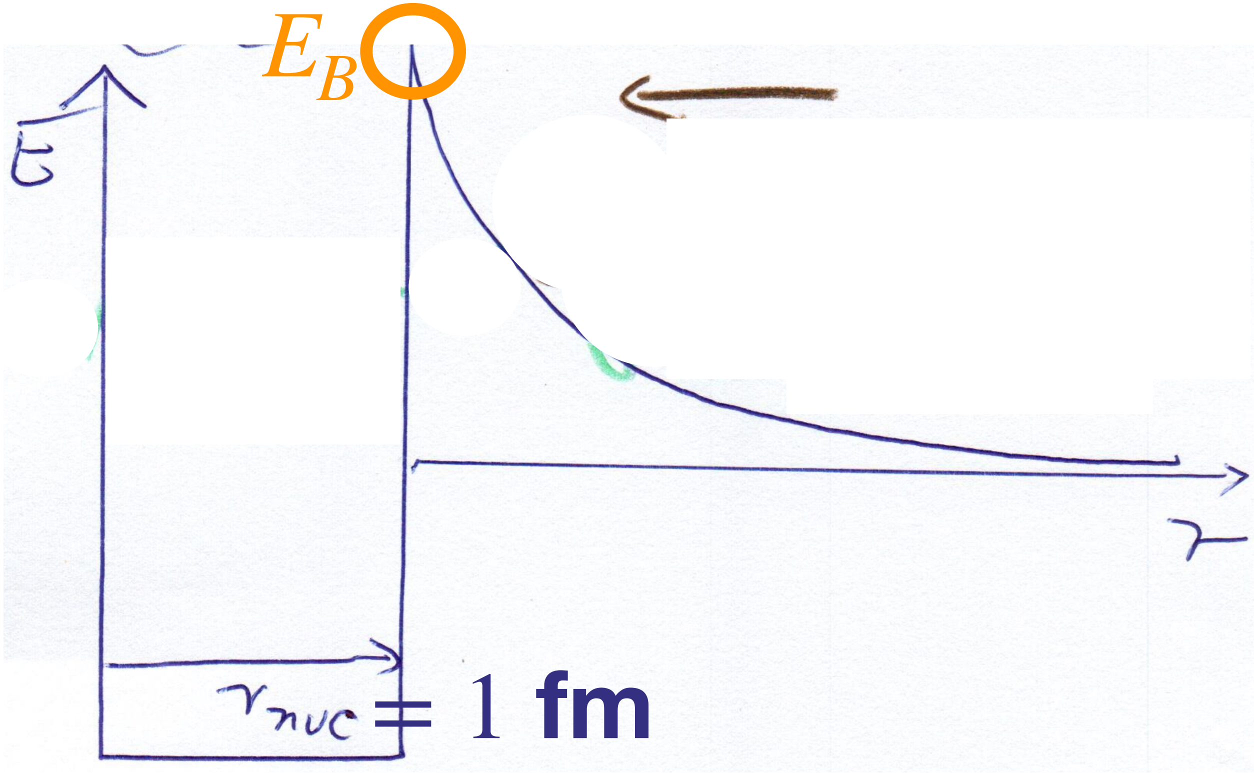


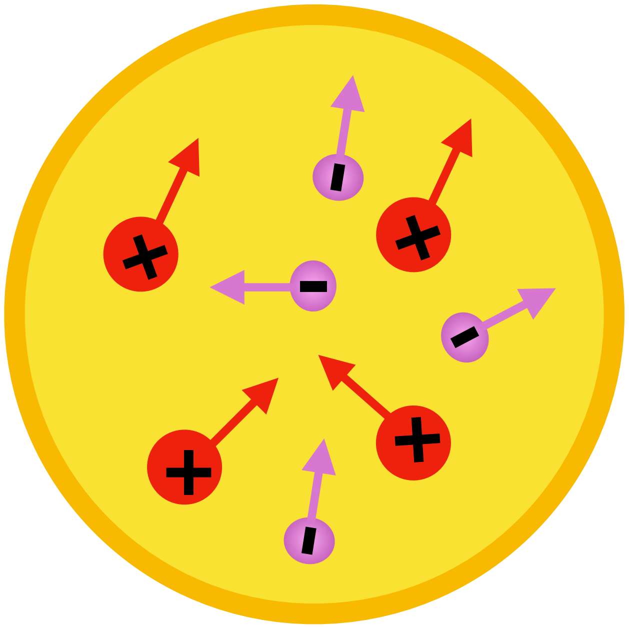
Example II: Nuclear fusion in the sun

- Barrier energy

$$E_B = \frac{e^2}{4\pi\epsilon_0 r_{nuc}}$$

$$= 1.4 \text{ MeV}$$





- Mean thermal energy Eq. (21) can reach this at a temperature

$$T \approx 10^{10} \text{ K}$$

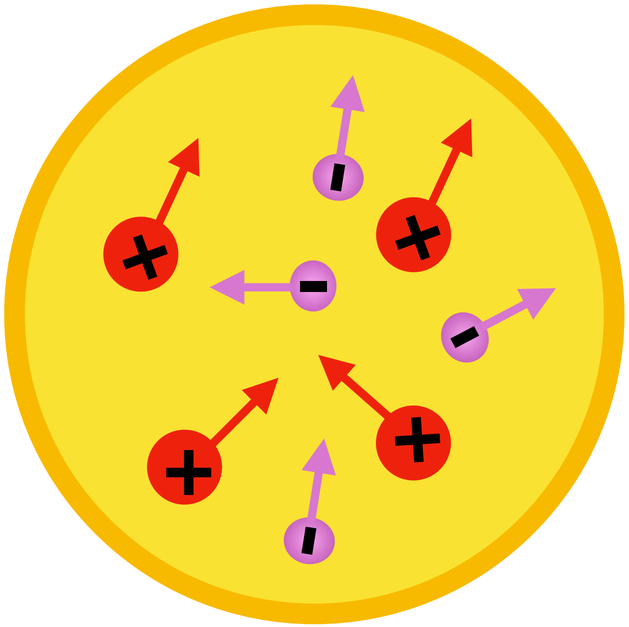
- Solar core "only"

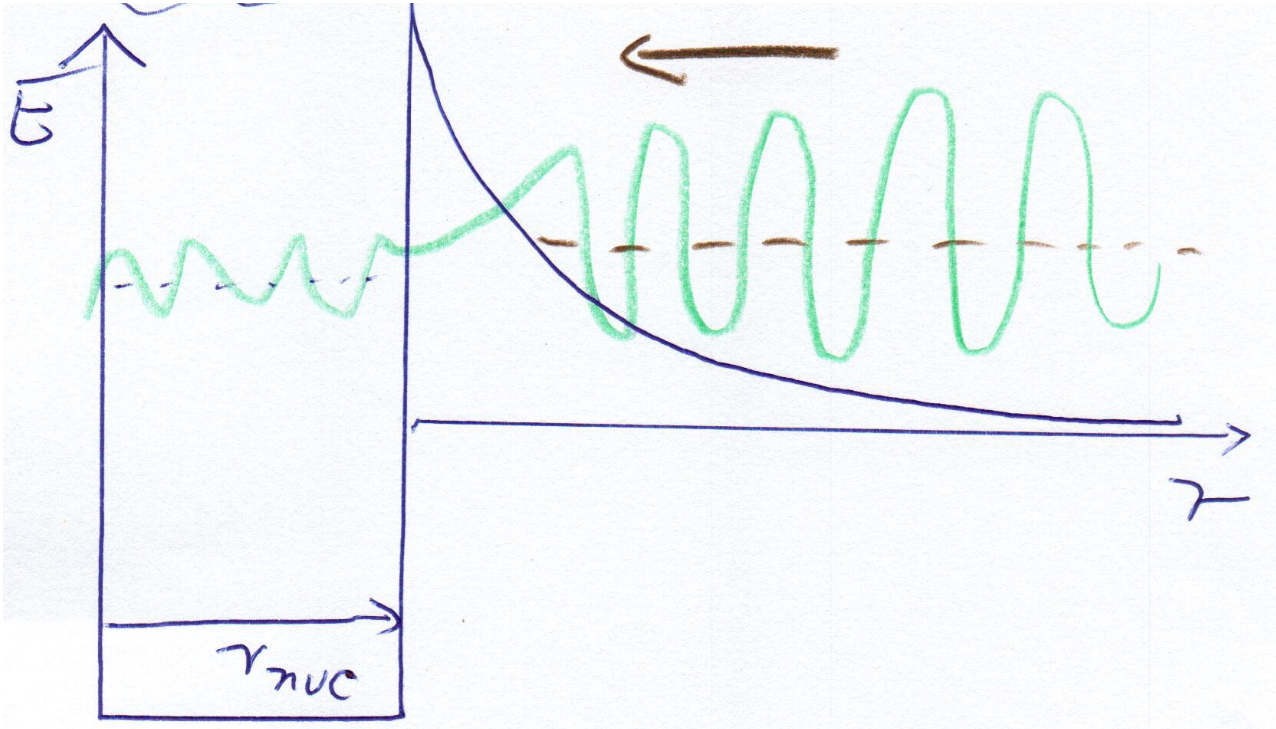
$$T \approx 1.5 \times 10^7 \text{ K}$$

Example II: Nuclear fusion in the sun

- With those numbers, it would be extremely unlikely to get a proton to fuse with another.

- But, luckily, the required energy is substantially reduced since proton can **tunnel** to its partner



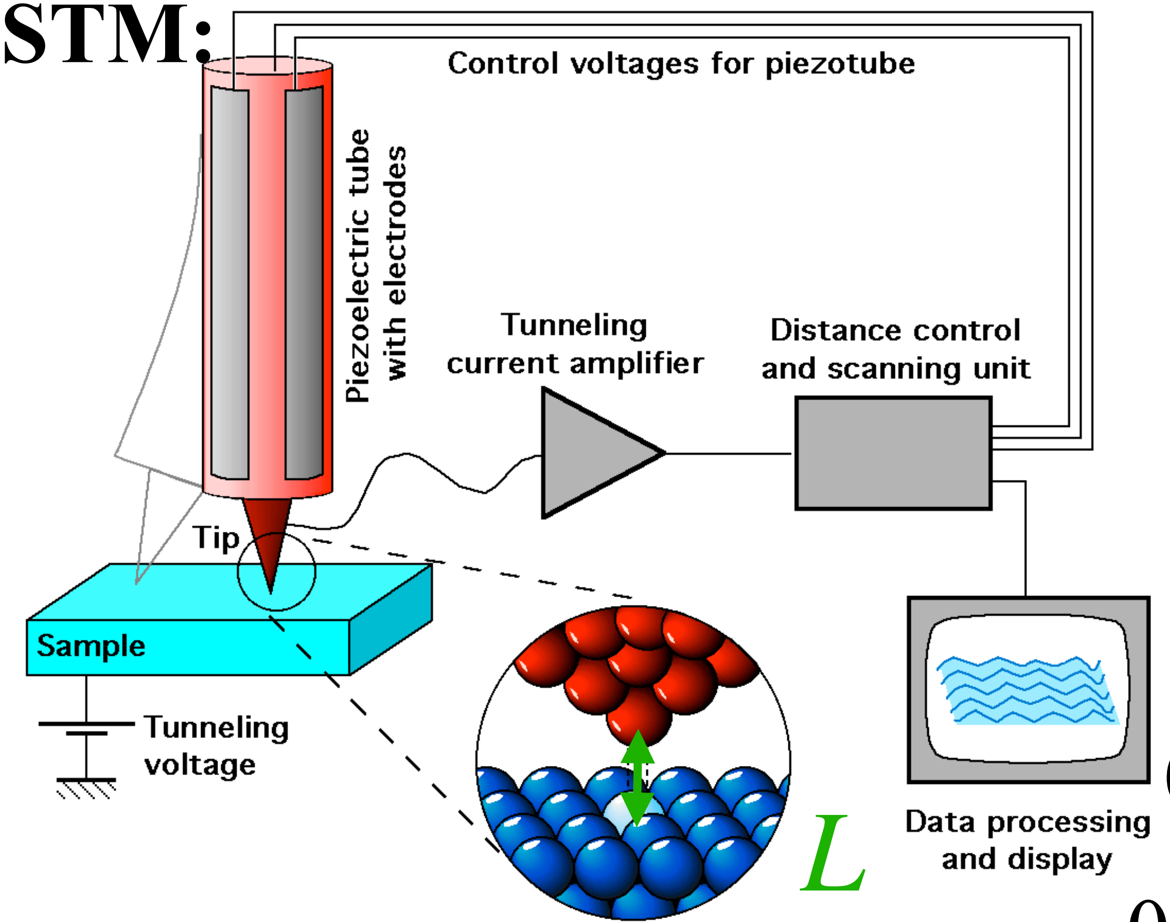


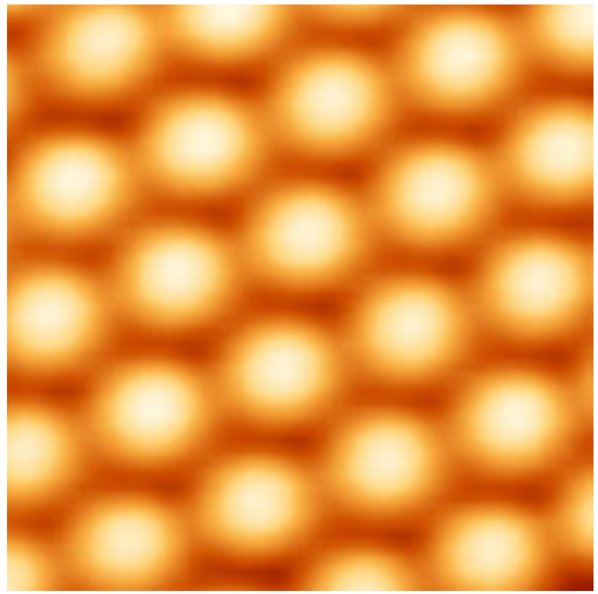
Example III: Scanning tunnelling microscope

- Exponential tunneling probability $T = e^{-2\kappa L}$

$\Longrightarrow$ very high sensitivity to L

STM:



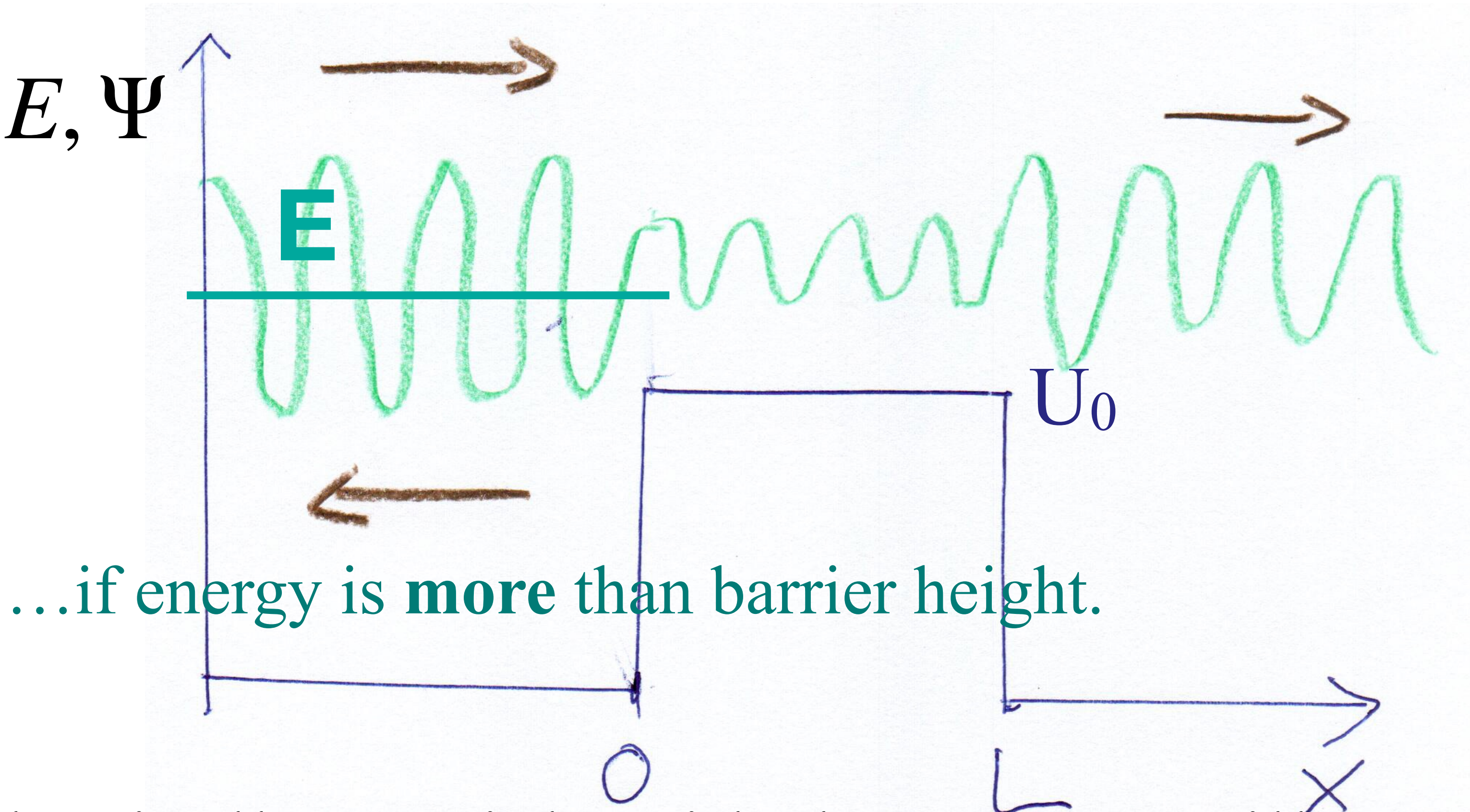


0.1 nm lateral resolution

0.01 nm depth resolution

3.3.3) Quantum reflection

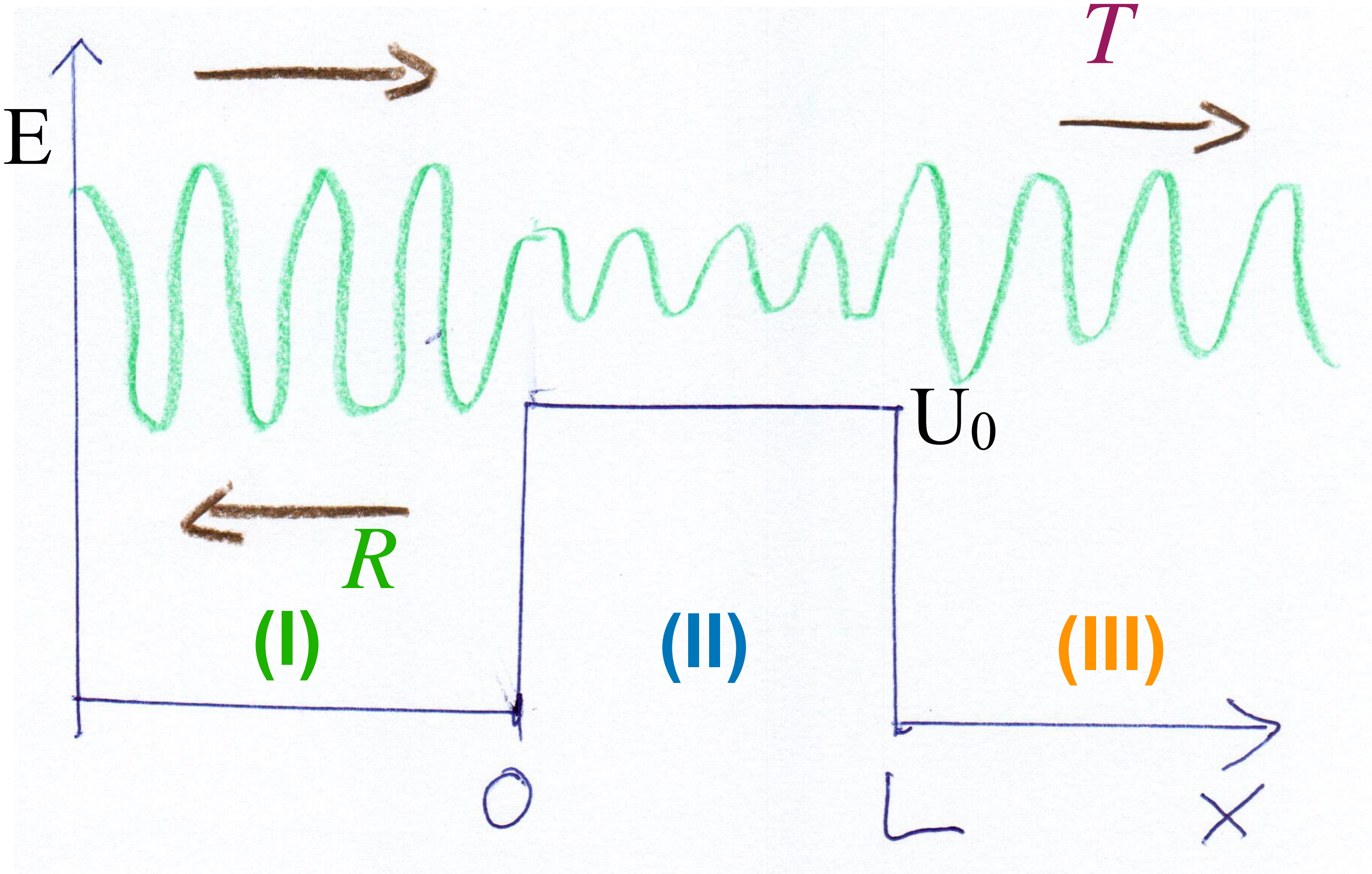
Let us now consider the same potential as in 3.3.2) but with energies E>U



Classically, particle with that energy will **always** pass barrier. Quantum?

Quantum reflection

Again our three region calculation



We find

Quantum reflection (114)

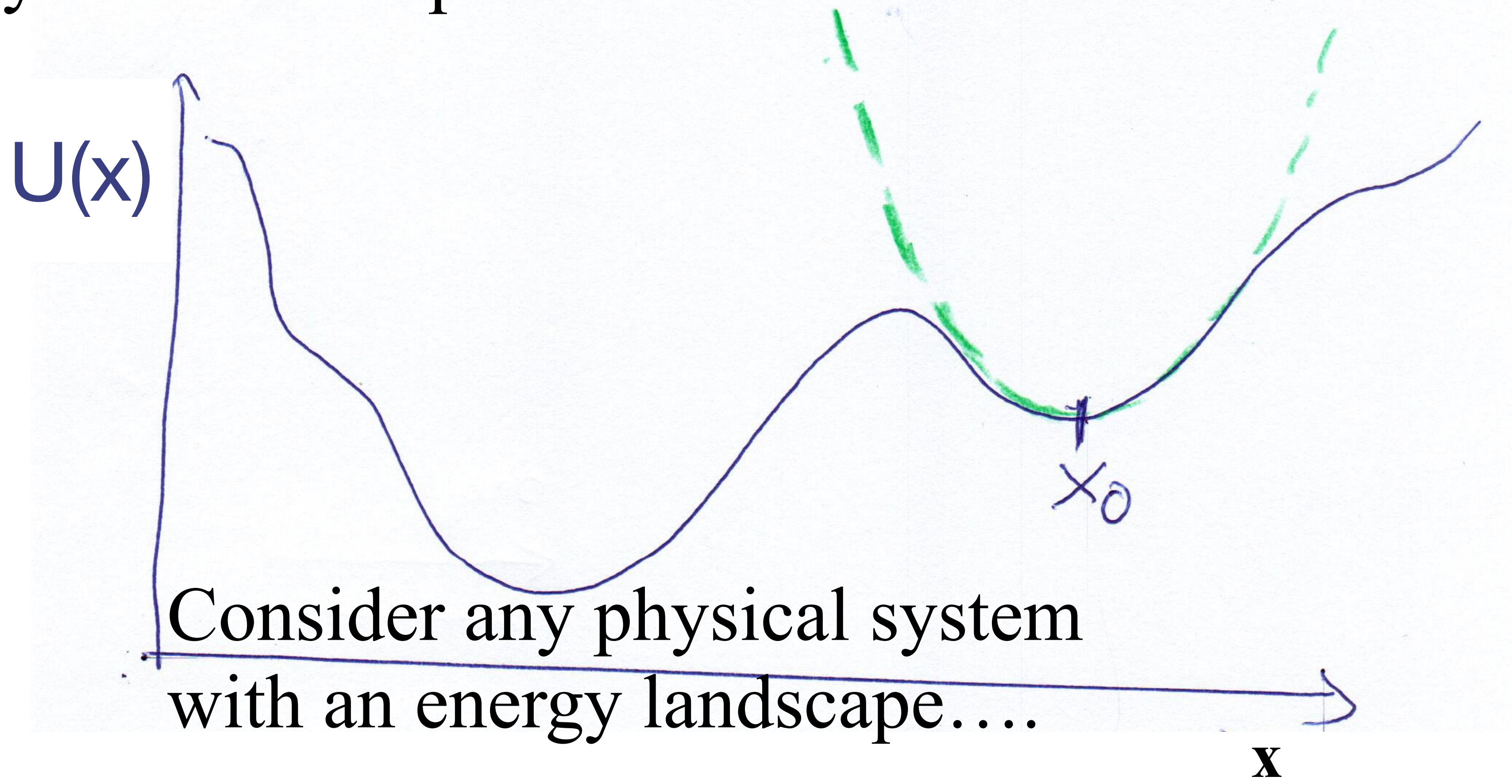
$R > 0,\ T < 1$ for reflection of a barrier even if $E > U_0$

3.3.4) The *Quantum* Harmonic Oscillator

We had started this lecture with the classical harmonic oscillator

near equilibrium this is a harmonic oscillator

Q: Why is HO so important?

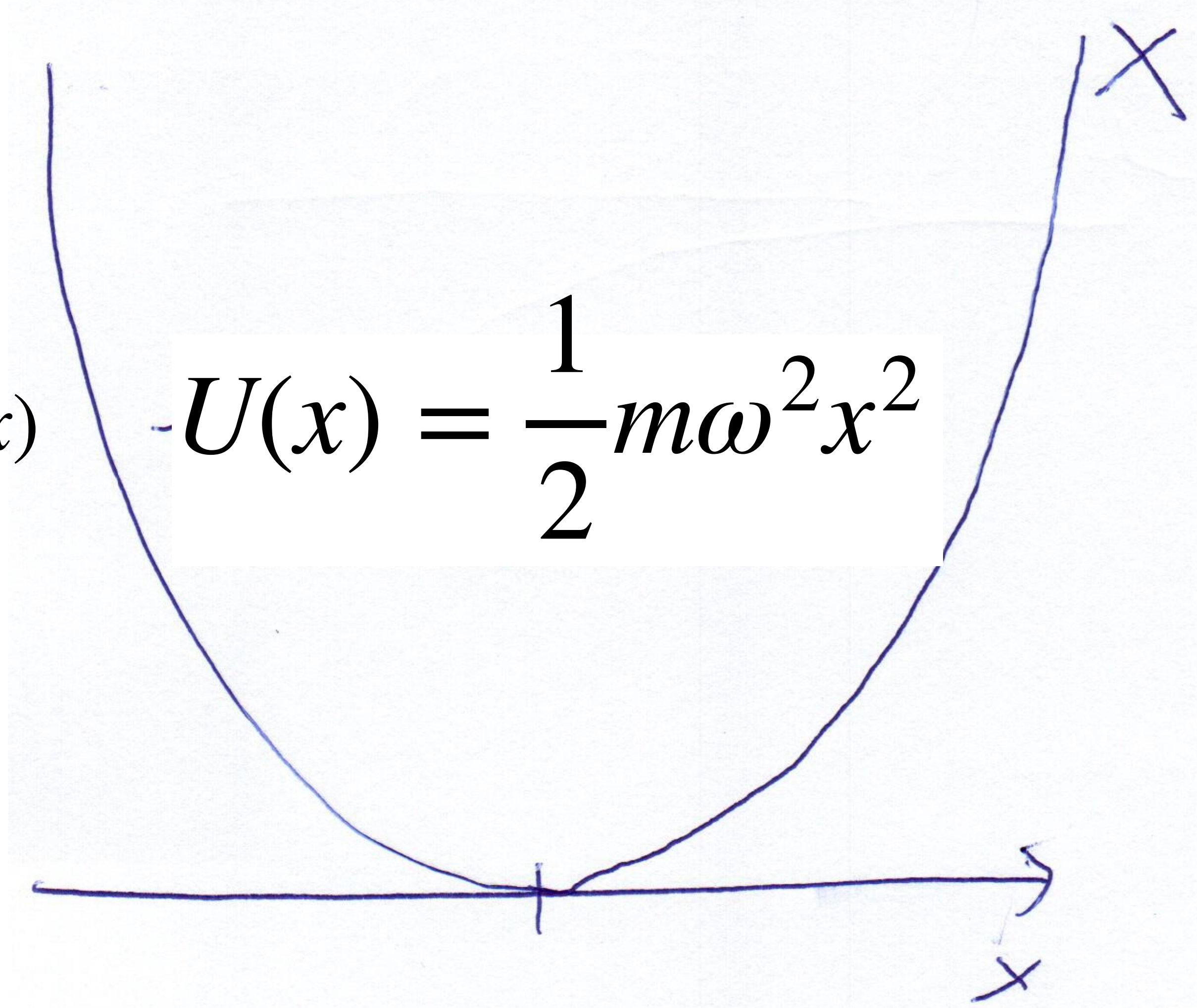


Consider any physical system with an energy landscape….

The *Quantum* Harmonic Oscillator

Now let the potential for the particle *U(x)* be

$$U(x) = \frac{1}{2} m\omega^2 x^2$$



Newton's Eq.

c.f. section 1.2.)

$$m \frac{d^2}{dt^2} x(t) = -\frac{d}{dx} U(x)$$

$$m \frac{d^2}{dt^2} x(t) = -m\omega^2 x$$

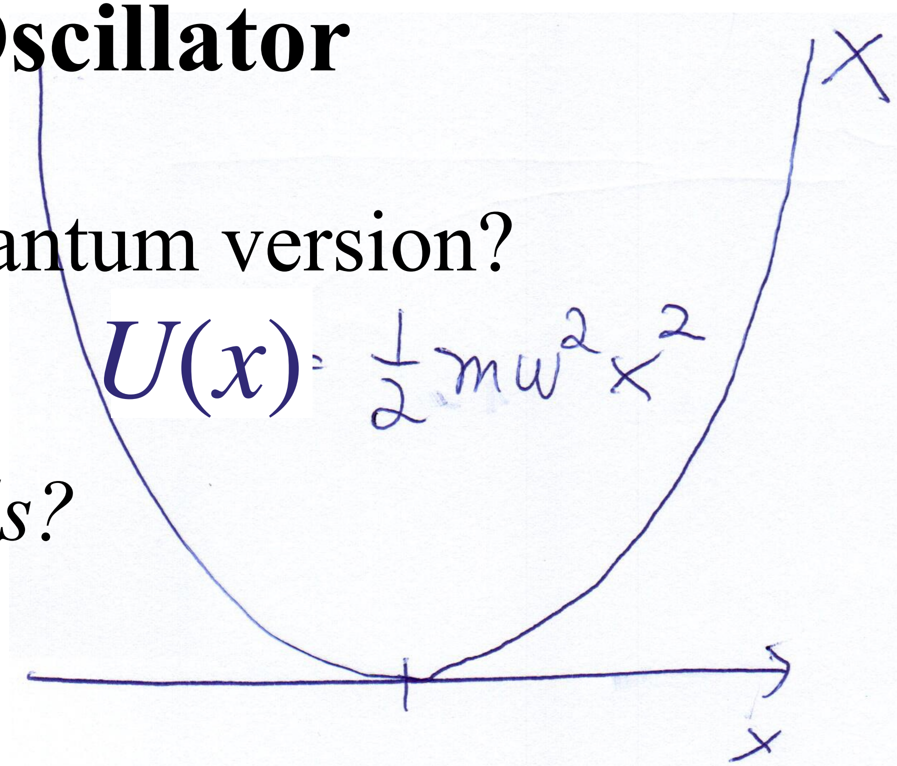
$$\frac{d^2}{dt^2} x(t) = -\omega^2 x$$

The *Quantum* Harmonic Oscillator

Can we now understand the quantum version?

Q: What do we expect?

A: Quantized energy levels?



Write again TISE:

$$E_n\phi_n(x) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2\right)\phi_n(x) \qquad \textbf{(115)}$$

Solution methods now more complicated. Turns out the normalisable solutions are…

(PHY 304)

The *Quantum* Harmonic Oscillator

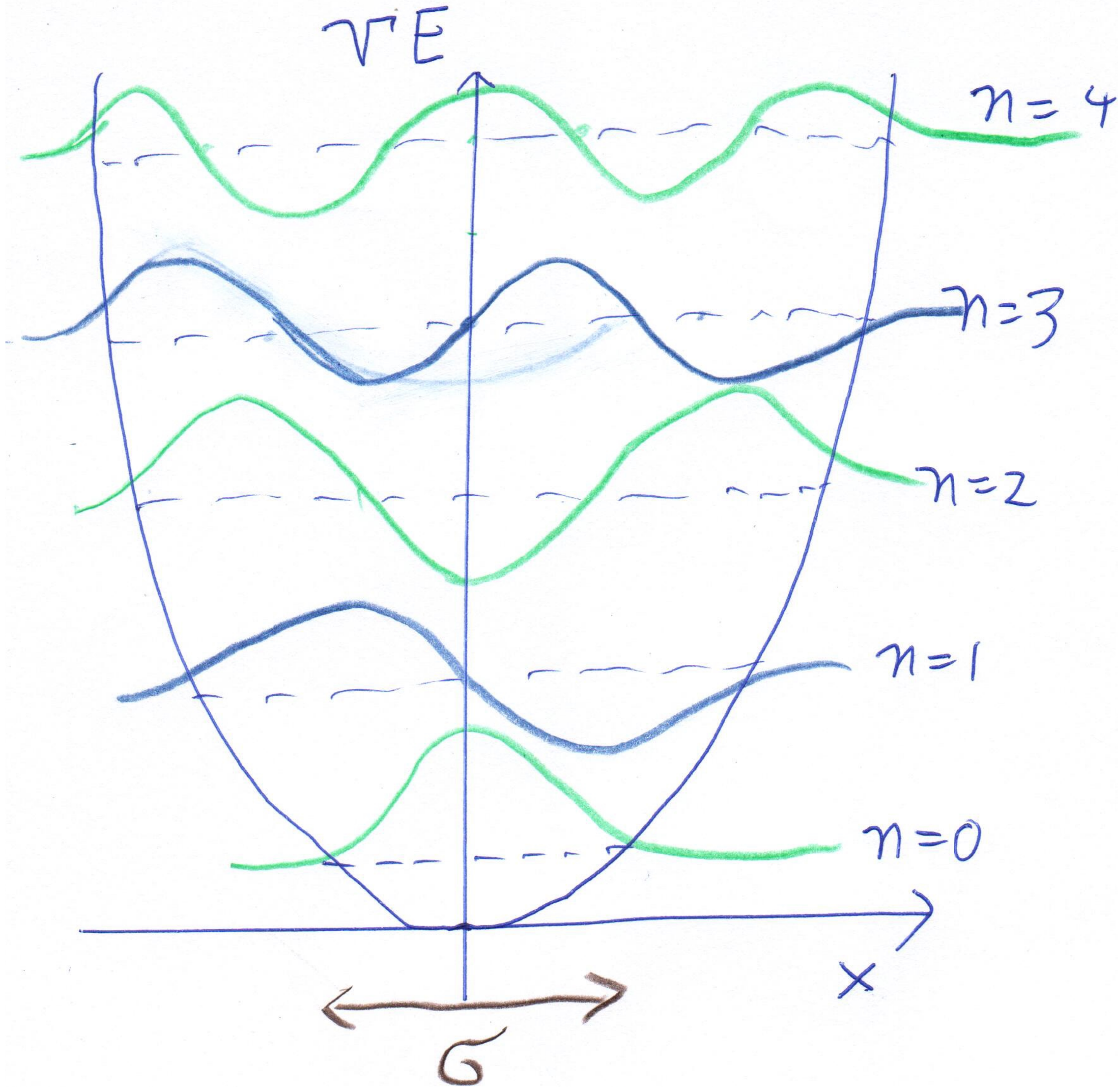
Solution of TISE for the harmonic oscillator

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) \qquad \phi_n(x) = \mathcal{N} H_n(x/\sigma) e^{-\frac{x^2}{2\sigma^2}}$$

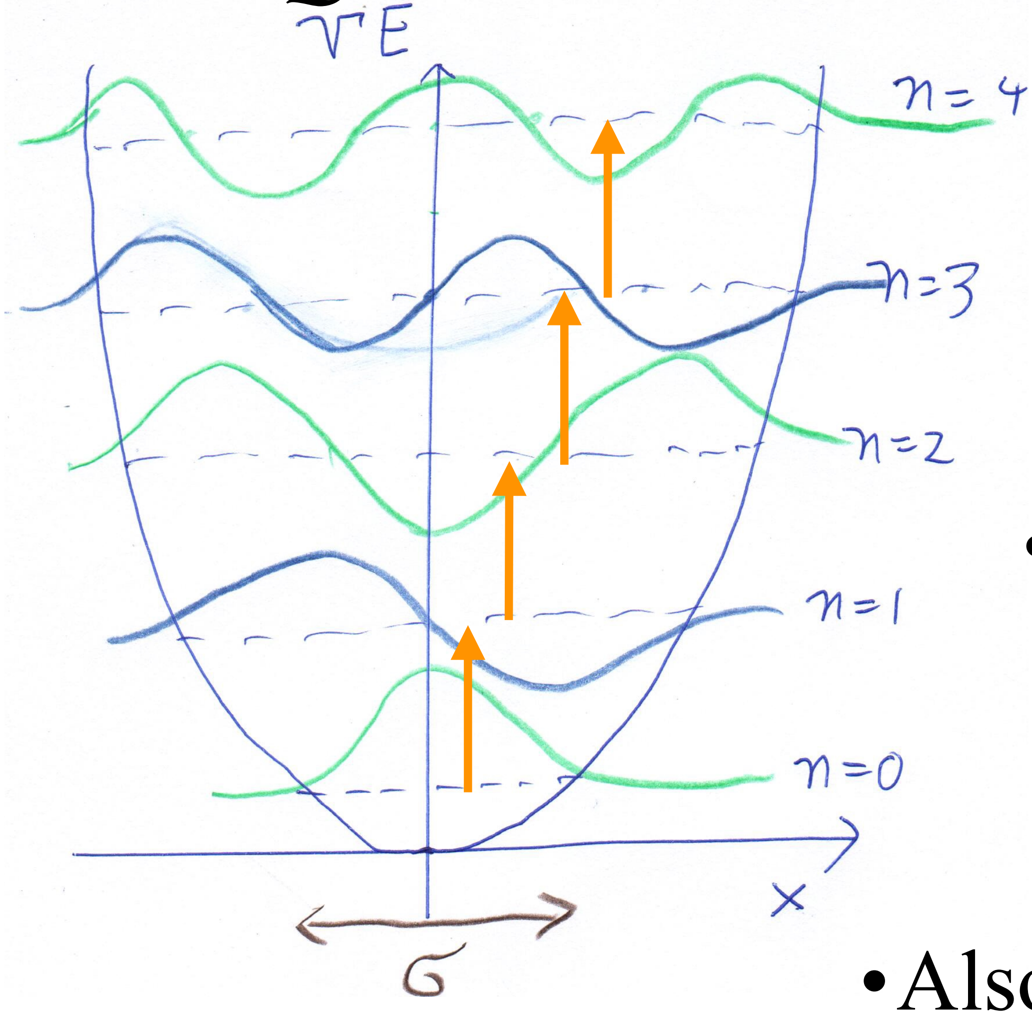
$$n = 0,1,2,\ldots \qquad \sigma = \sqrt{\frac{\hbar}{m\omega}} \qquad (116)$$

- As seen before, the oscillator has some minimal energy, called **zero-point energy**: $E_0 = \frac{\hbar\omega}{2}$ **(117)**
- $H_n(x)$ are special functions called **Hermite-polynomials**. $\mathcal{N}$ is a normalisation factor.
- $H_0(x) = 1$, hence the ground-state wave function $\phi_0(x)$ is a **Gaussian**, with zero-point width σ

The *Quantum* Harmonic Oscillator



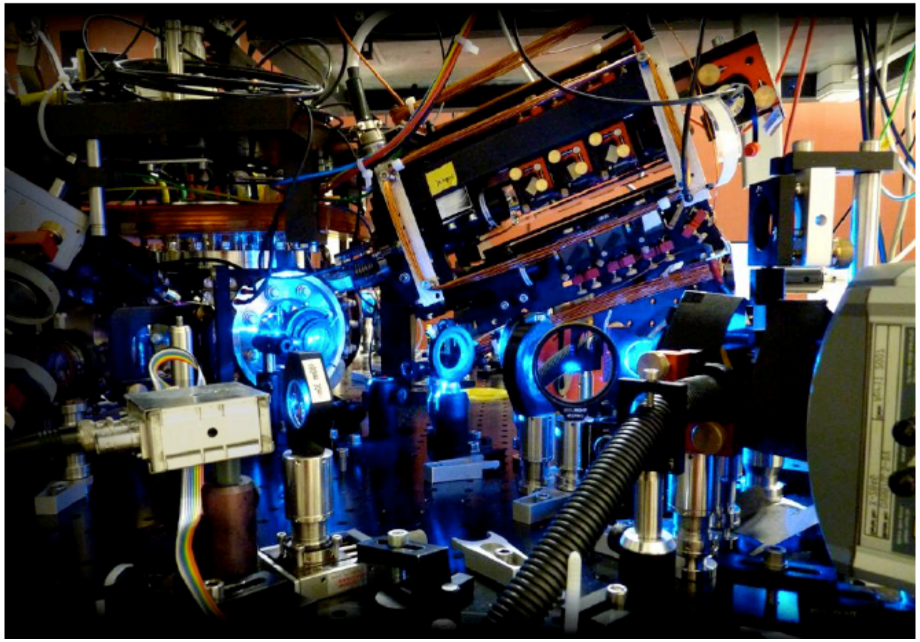
The *Quantum* Harmonic Oscillator



- Most important features is the **equal distance in energy** between all levels $\Delta E = E_{n+1} - E_n = \hbar\omega$
- Quantum manifestation of classical fact that oscillation frequency **does not** depend on amplitude
- Also implements resonance catastrophe: Excitation with quanta of energy ΔE can drive very high excitations

Example I:
Bose-Einstein condensate in an atom trap

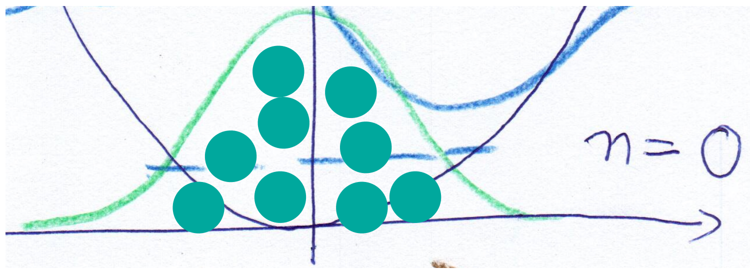
image courtesy Shannon Whitlock,
Uni Heidelberg / Strassbourg



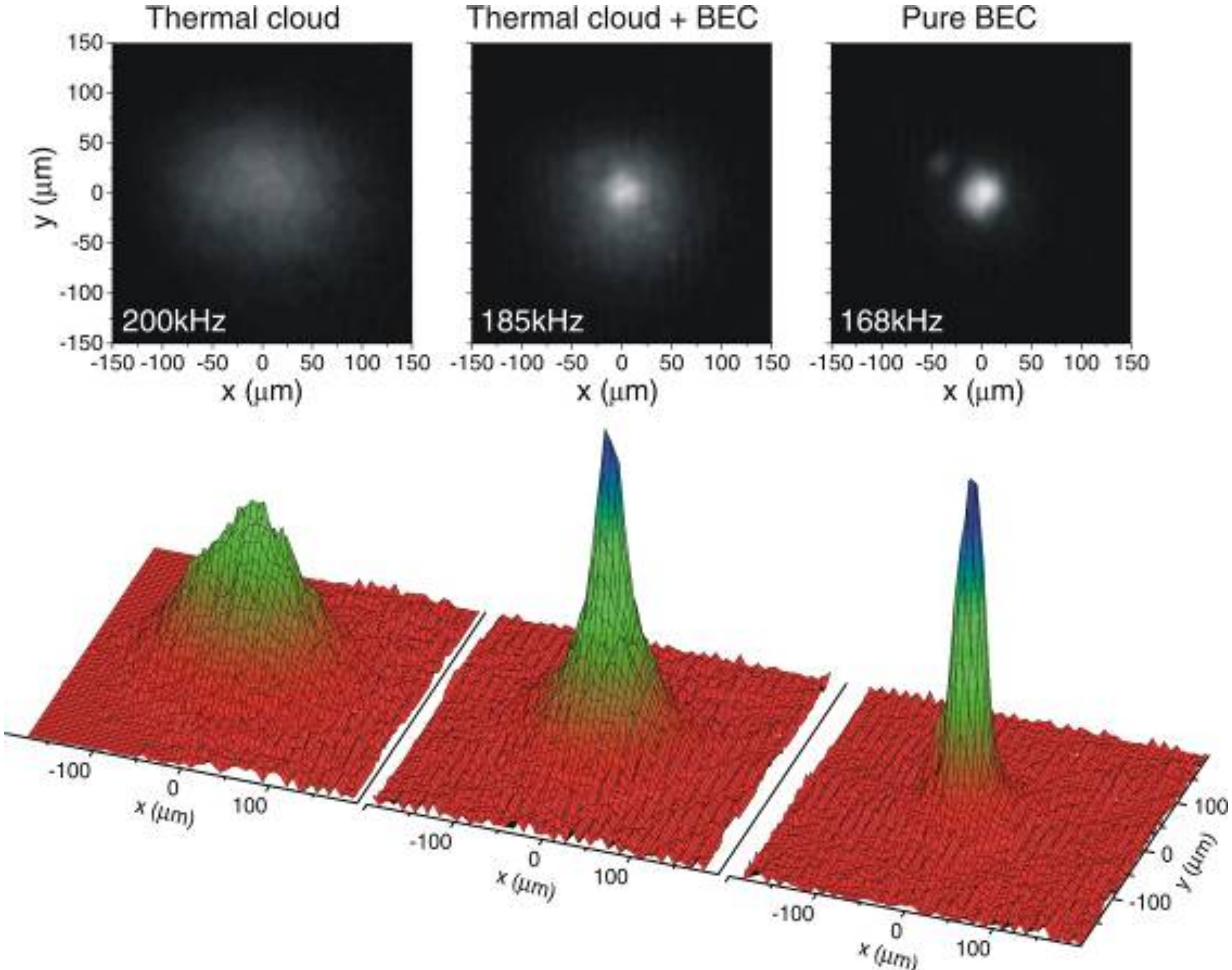
Cool dilute gas of ^{87}Rb atoms **with lasers** while trapped

At lowest temperature, all atoms go into trap ground state $\phi_0(x)$
[in Eq. (116)]

Can now **see oscillator ground state** in **single** picture



Example I:
Bose-Einstein condensate in an atom trap

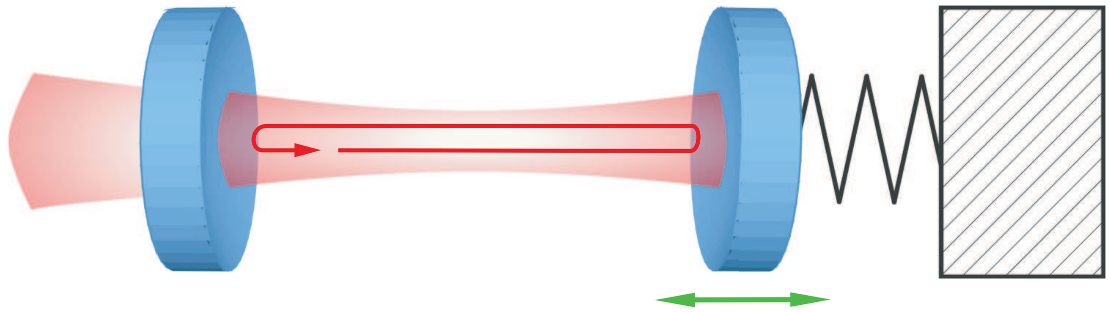


http://www-personal.umich.edu/~graithel/bose.html

Example II: Quantum-opto-mechanics
(large quantum oscillators)

Optical cavity with
vibrating end mirror:

(a)



Kippenberg and Vahala, Opt. Express **15** 17172 (2007).

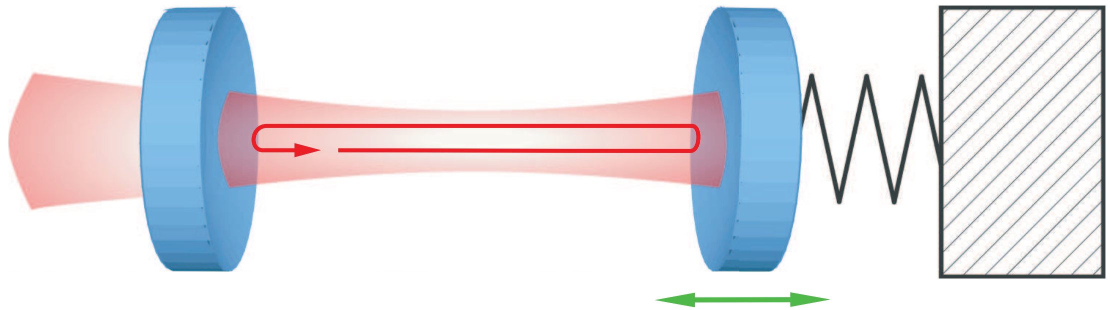
- Position of the mirror ⇒ wave length of standing waves in cavity via Eq. (16) **[mirror affects light]**
- Light intensity affects mirror position via radiation pressure, photon momentum , see section 2.2.5) **[light affects mirror]** (driven oscillator, section 1.2)

Example II: Quantum-opto-mechanics
(large quantum oscillators)

Optical cavity with vibrating end mirror:

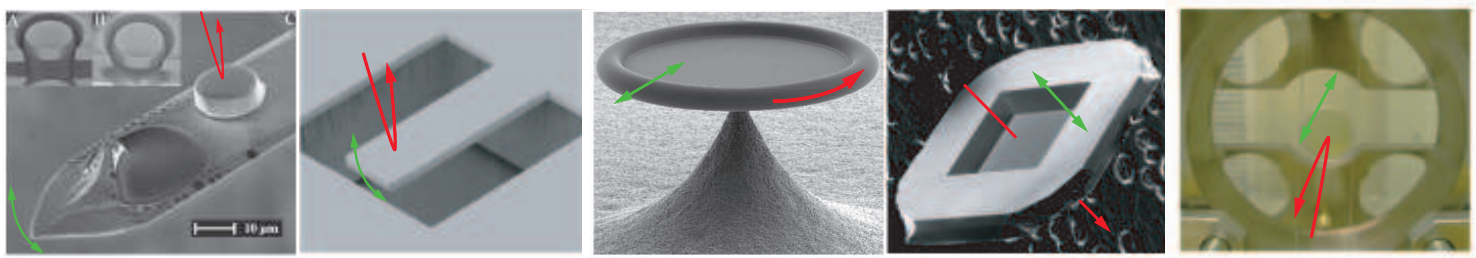
Oscillator driving force by light

(a)



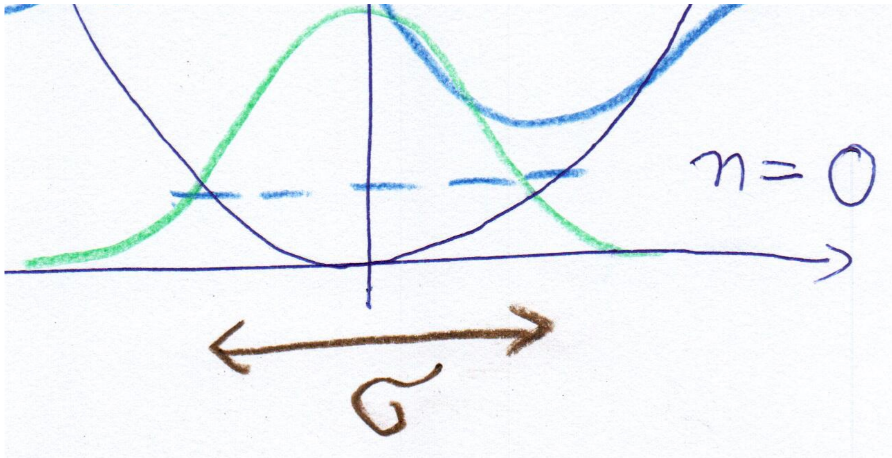
Kippenberg and Vahala, Opt. Express **15** 17172 (2007).

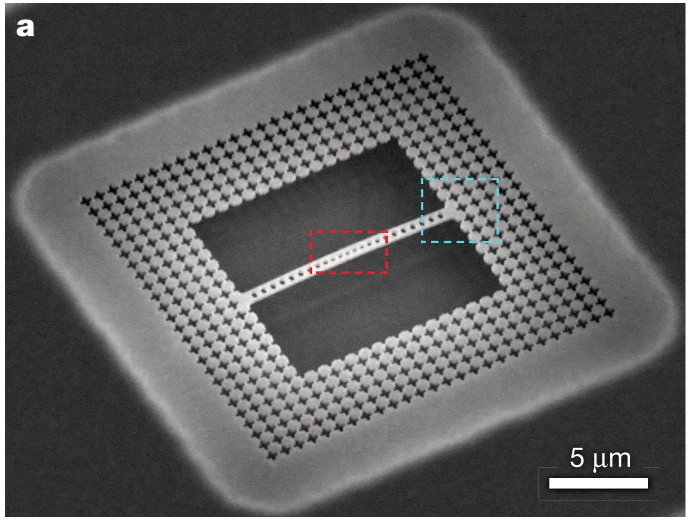
(b)



$\mathcal{F}$	200	30,000	22,000	15,000	4,000
$\Omega_m/2\pi$	12.5 kHz	814 kHz	57.8 MHz	134 kHz	12.7 Hz
Q_m	18,400	10,000	2,900	$1.1 \cdot 10^6$	19,950
m_{eff}	24 ng	190 μg	15 ng	40 ng	~1 g
Ref.	[34]	[26,27]	[22,28]	[30]	[29]

Example II: Quantum-opto-mechanics
(large quantum oscillators)





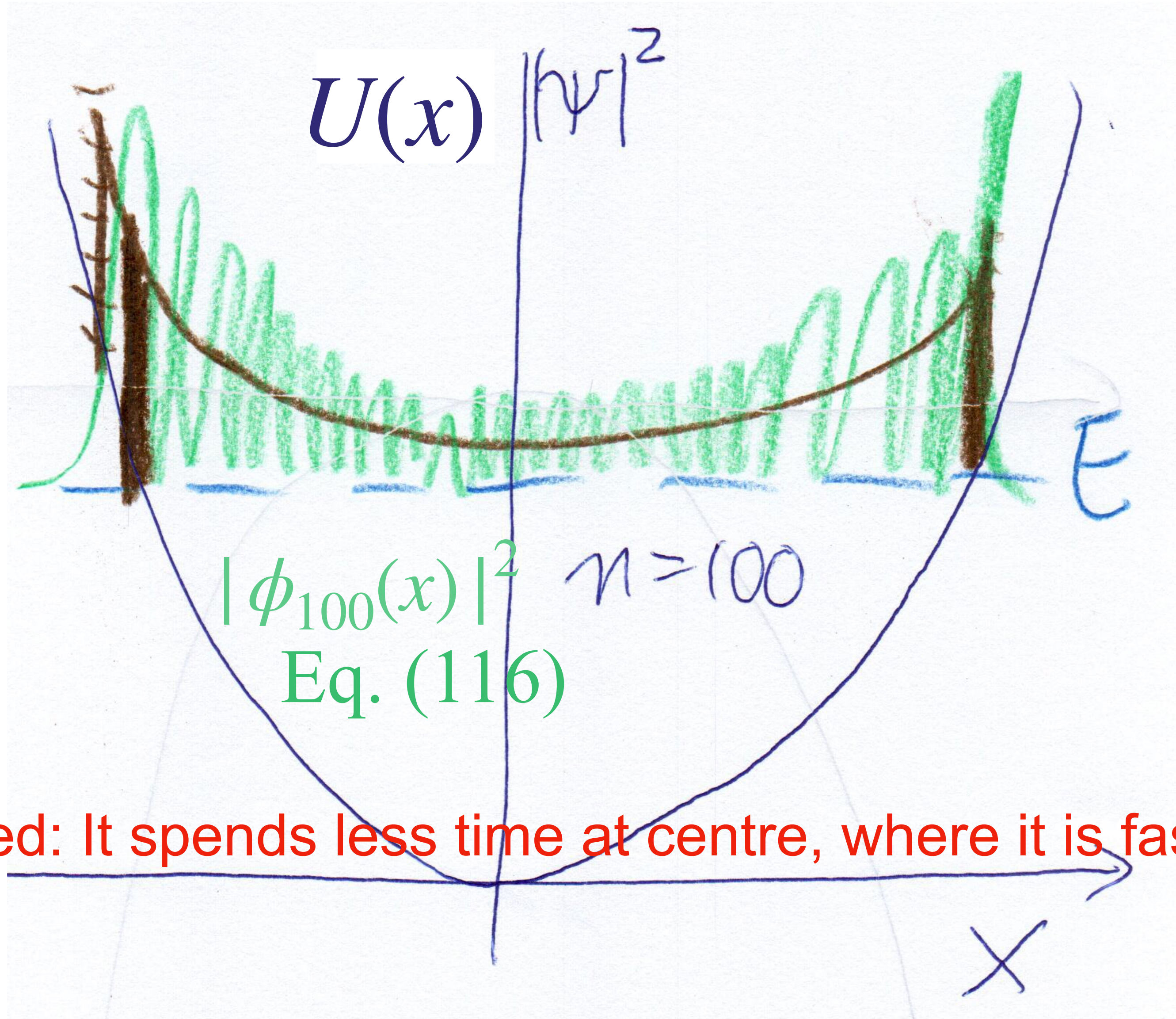
- Succeeds to **cool** nano-mechanical oscillator of mass $m = 311$ **fg** $= 3.1 \times 10^{-18}$ **kg** to almost its quantum mechanical **oscillator ground state** $n = 0$ in Eq. (116).

J. Chan *et al.*, Nature **478** 89 (2011).

3.3.5) The correspondence principle

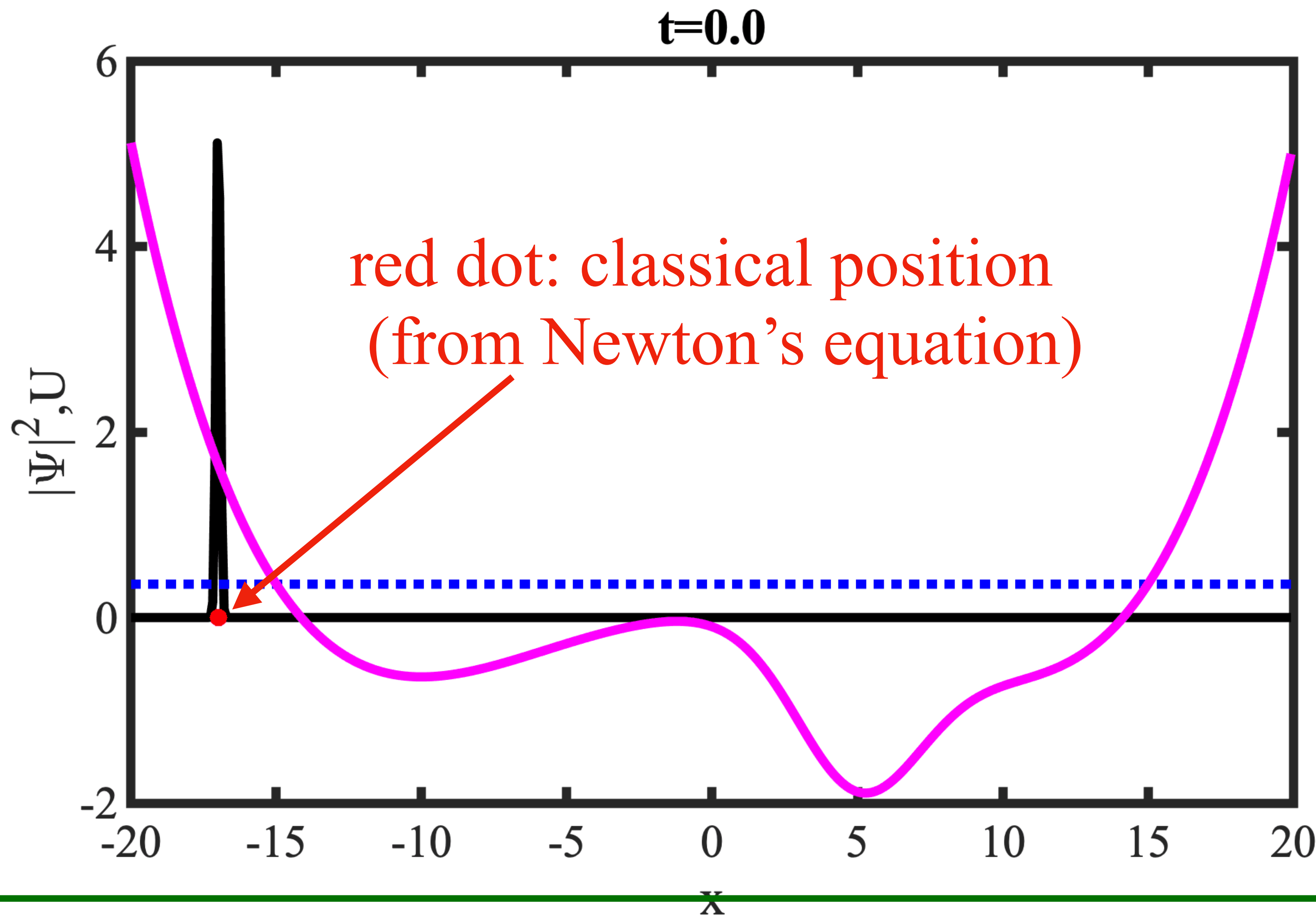
Let us again re-visit the correspondence principle (3.1.9)

For large n, spatial average of $|\phi_n(x)|^2$ gives the classical probability distribution of the harmonic oscillator (brown line) [Time averaged: It spends less time at centre, where it is fast]



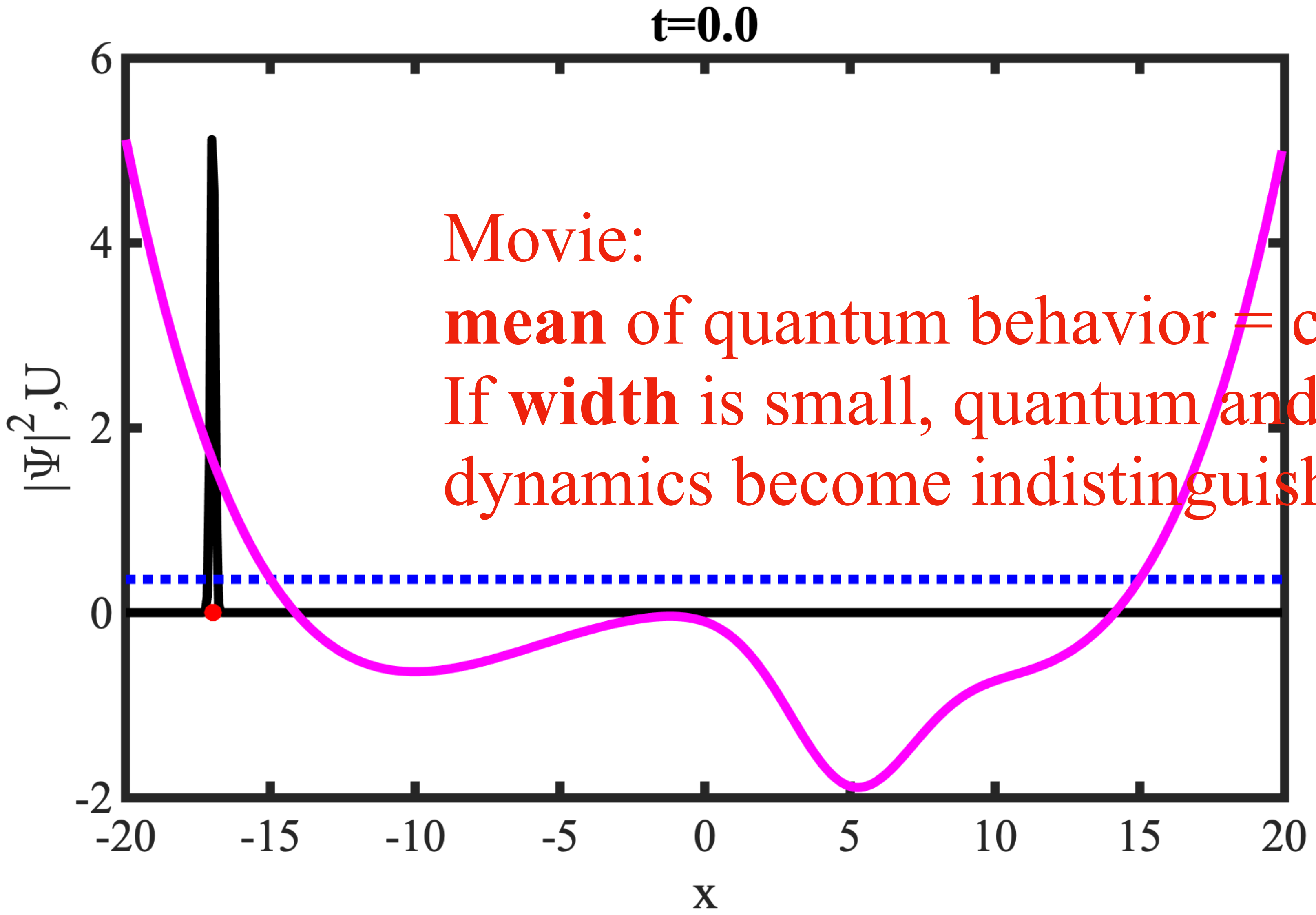
Example: The correspondence principle

Same as example section 3.2.1, but mass *=2000, and much narrower wavepacket



Example: The correspondence principle

Same as example section 3.2.1, but mass *=2000, and much narrower wavepacket



Movie:
mean of quantum behavior = classical.
If **width** is small, quantum and classical dynamics become indistinguishable.