Quantum Physics 1

2015-2016

These slides: Wave Mechanics and Solid State

Lectures for the 8th week of the course

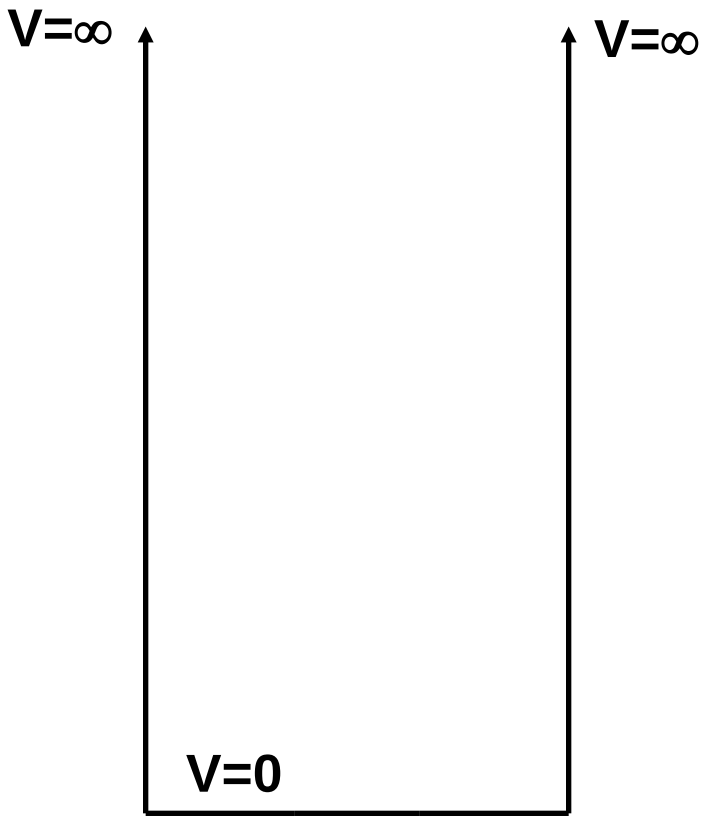
This week mainly re-visit Chapter 2 and solid-state physics topics of Chapter 5

Any questions on the material till now?

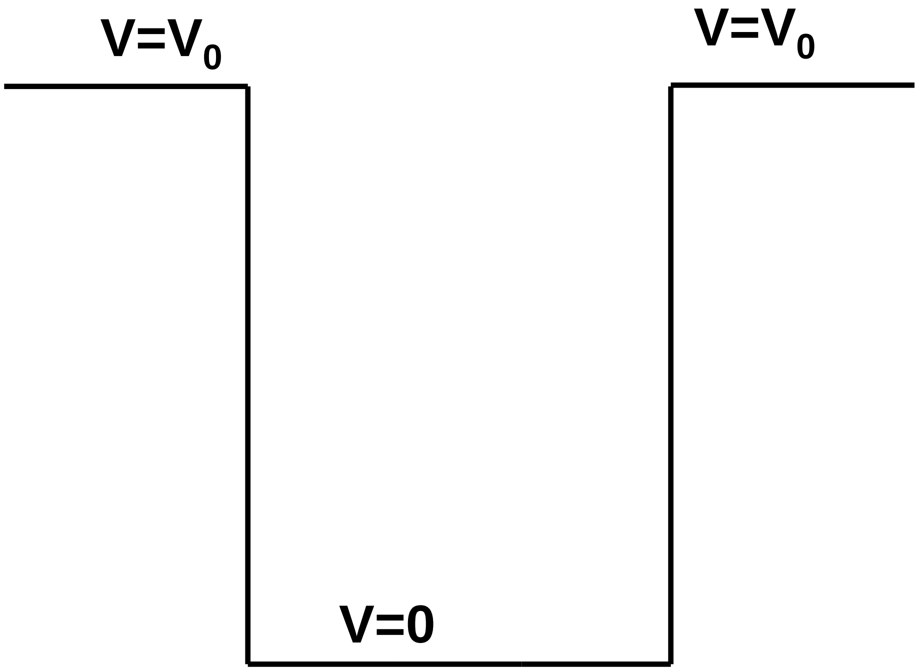
This week (many parts done on the board)

1. Wave mechanics
2. Tunneling
3. Weakly coupling 2, 3, many quantum systems
4. From particle-in-a-well to solid state physics

Until now:



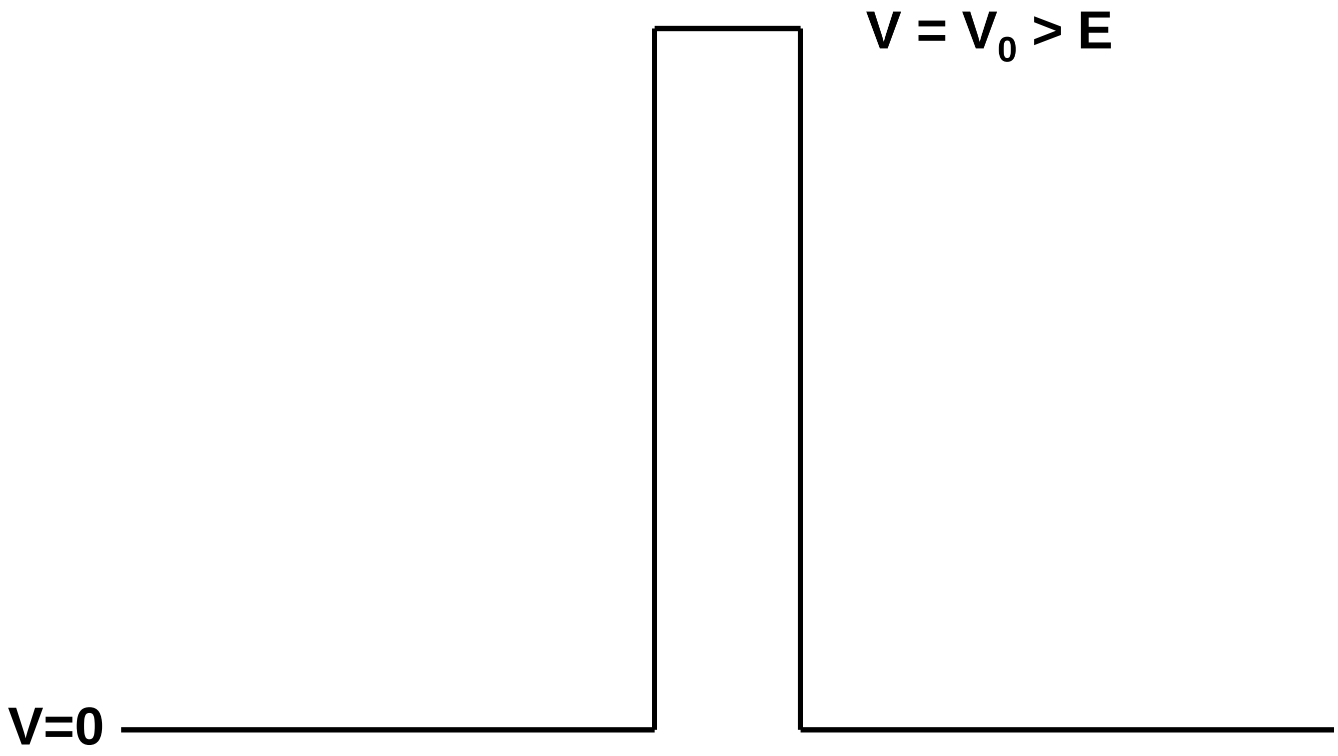
More realistic:



What are now the energy eigenfunctions and eigenvalues?

Tunnel effect

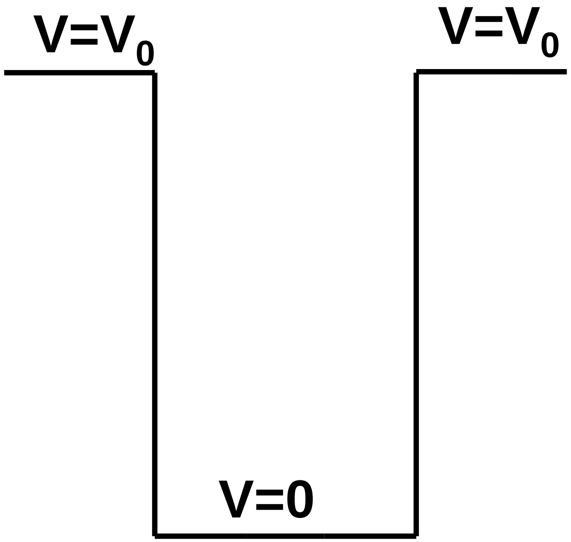
What is the behavior of a matter wave coming in form the left?

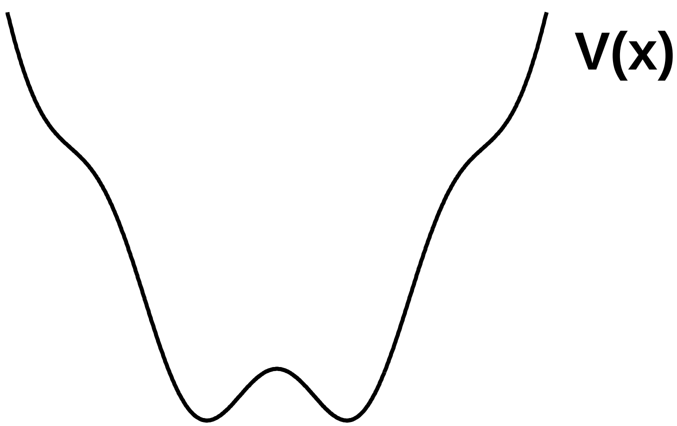


Griffiths book problem 2.33

Two cases

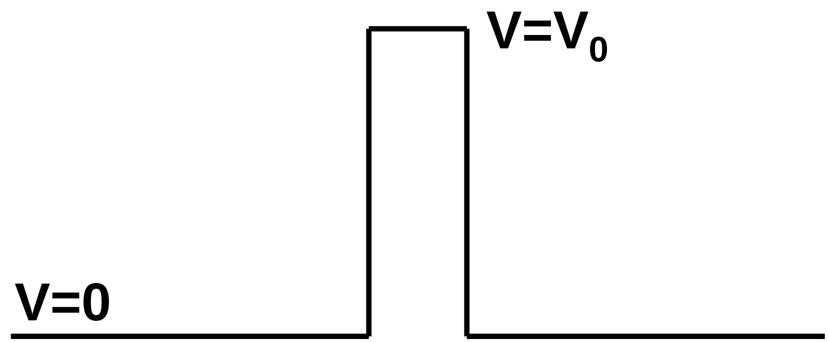
Confined systems



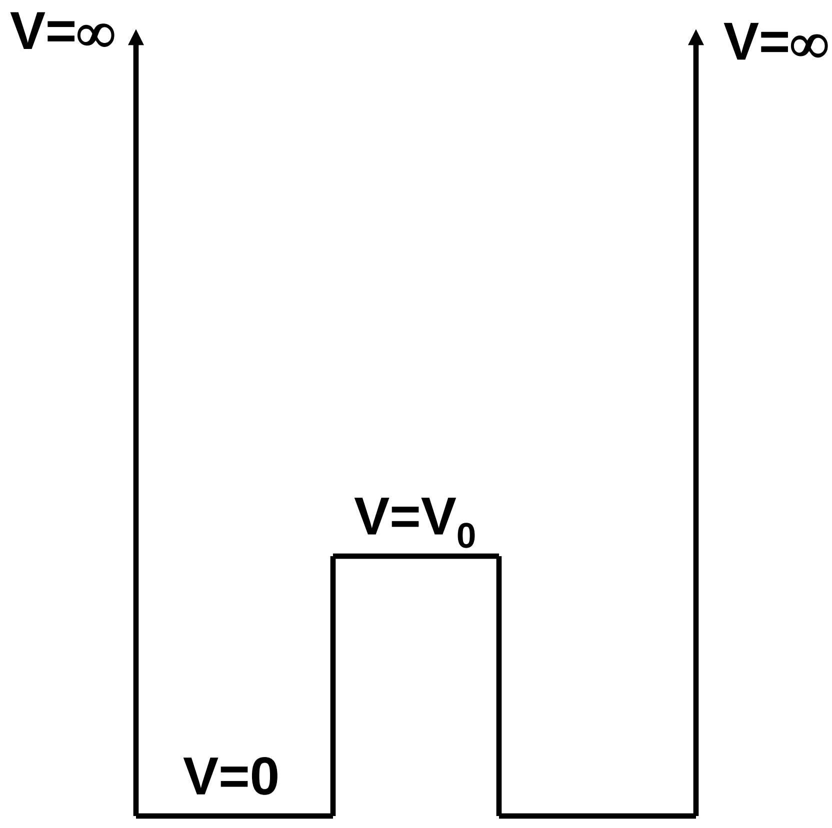


Scattering

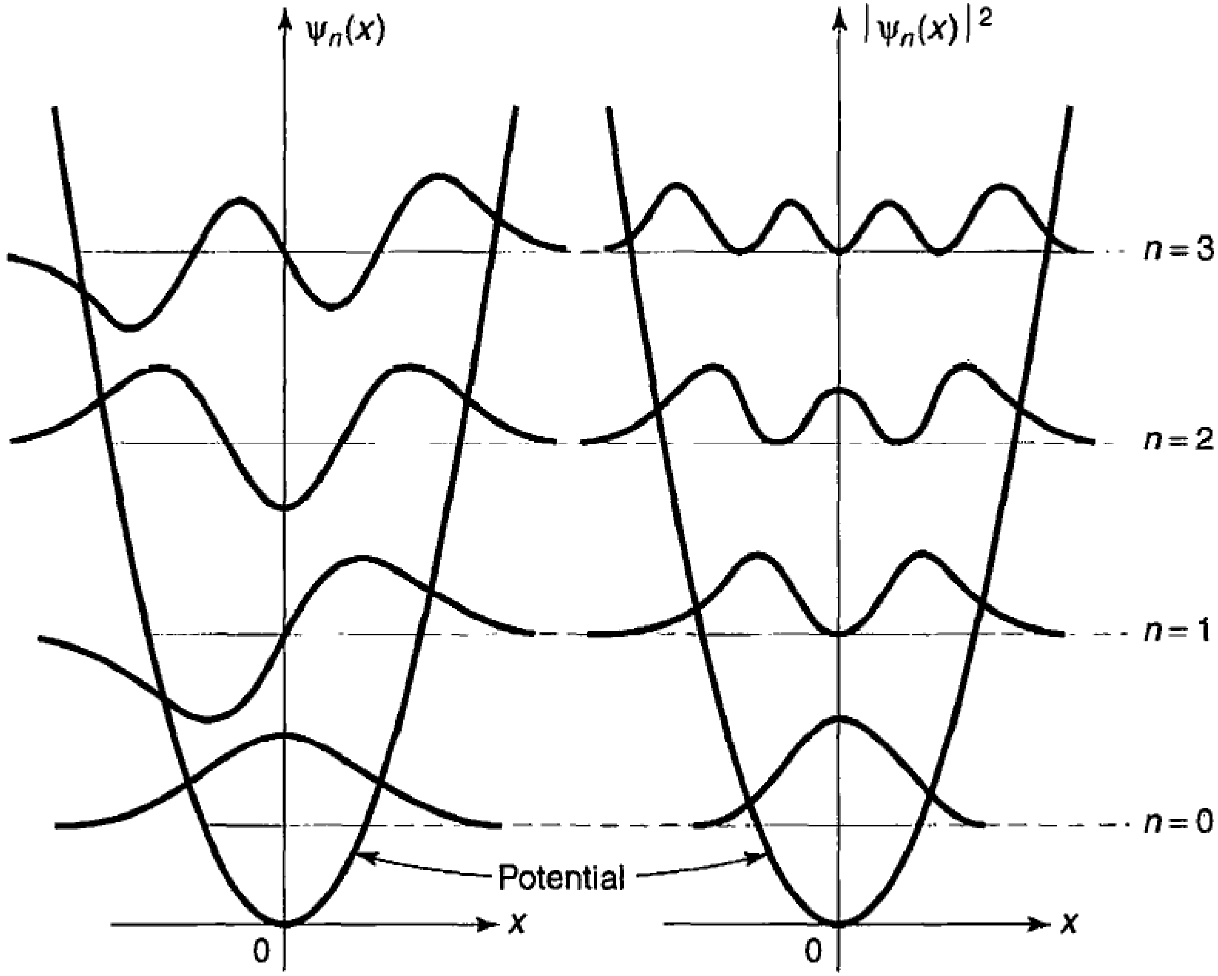
$V_0 > E$ and $V_0 < E$ both relevant



What is the wavefunction for the ground state?
(………this is beginning of SOLID STATE PHYSICS)



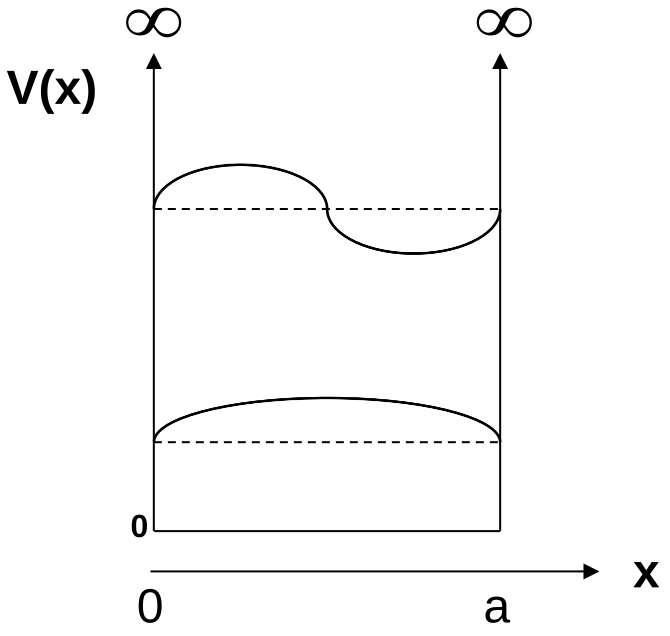
Griffiths book Fig. 2.7



Peer instruction question

How many graphs do you see at the same time here?

A 1
B 2
C 3
D 4



Time-independent Schrodinger equation:

$$\hat{H} = \hat{T} + \hat{V}$$

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \hat{V}(x)$$

$$\hat{H}\left|\varphi_n\right\rangle = E_n\left|\varphi_n\right\rangle$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\varphi_n(x) + \hat{V}(x)\varphi_n(x) = E_n\varphi_n(x)$$

$$\frac{\partial^2}{\partial x^2}\varphi_n(x) = -k^2\varphi_n(x)$$

$$k = \sqrt{\frac{2m(E-V)}{\hbar^2}} \qquad \text{for } E > V \text{ with } \; e^{\pm ikx} \text{ solutions}$$

$$or \qquad k' = \sqrt{\frac{2m(V-E)}{\hbar^2}} \qquad \text{for } V > E \text{ with } \; e^{\pm k'x} \text{ solutions}$$

Solving eigenfunctions:
General case for time-independent Hamiltonian

Philisophy for various sections with different constant V(x)
Harmonic Oscilator => similar for non-constant V(x)

To find Ψ for realistic physical situation, use these boundary conditions (here 1D case):

Question 1, why these items 1 & 2?
Otherwise…..

A state cannot be normalized.
B Schrödinger eq. cannot be solved.
C too much kinetic energy needed.
D it would require V(x) to be infinitely steep

1. Ψ continuous
2. dΨ/dx continuous
3. Ψ normalized $\int \Psi^*\Psi \, dx = 1$
4. Ψ limited, no unphysical extremes
5. Ψ is single-valued

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General case for time-independent Hamiltonian
Philisophy for various sections with different constant V(x)
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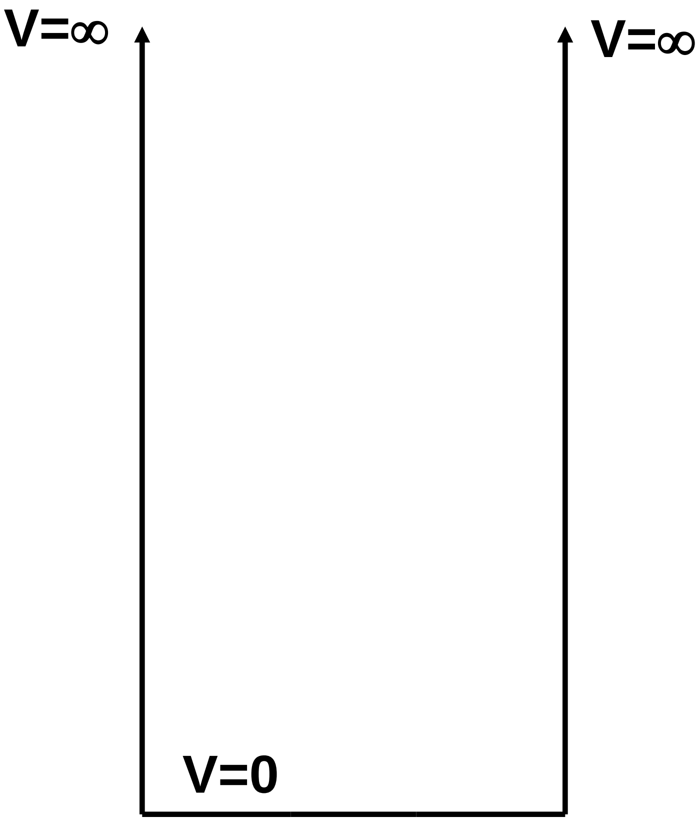
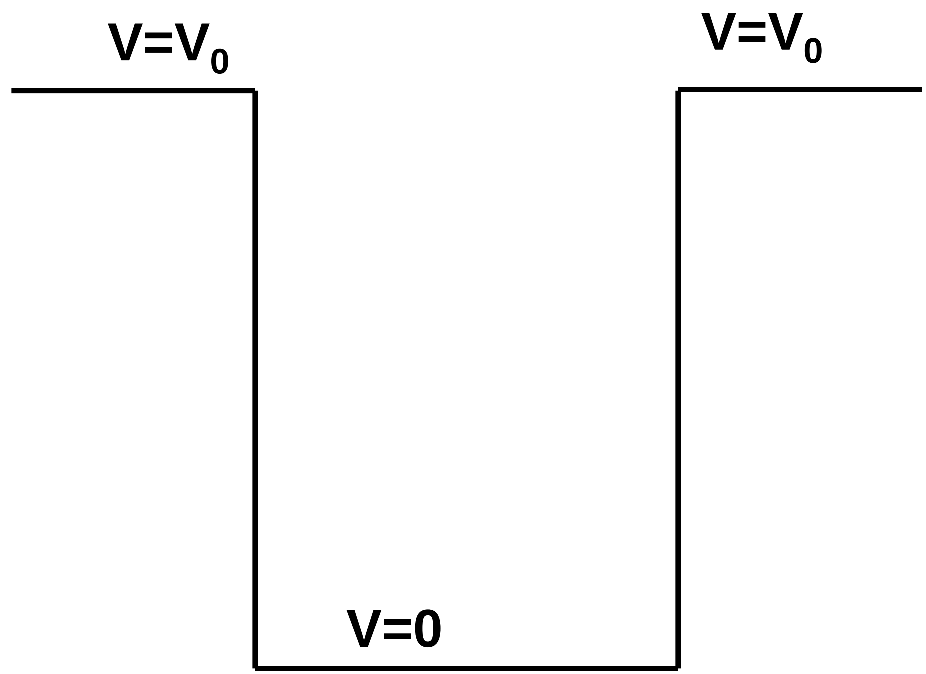
} (for 1 and 2) Otherwise Fourier components with extremely high kinetic energy (high k-values) needed to form Ψ

Until now:

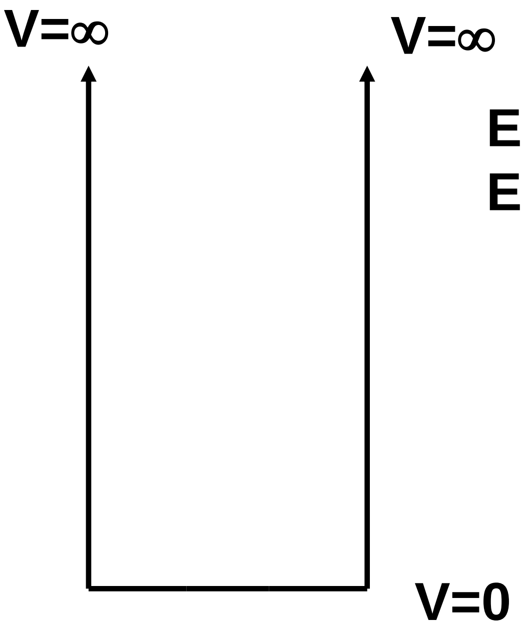


More realistic:



What are now the energy eigenfunctions and eigenvalues?

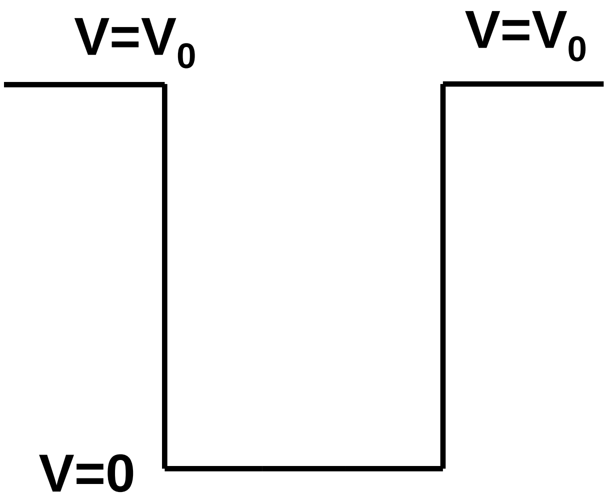
Infinite



$E_n = n^2 E_1$

$E_1 = \hbar^2\pi^2/2ma^2$

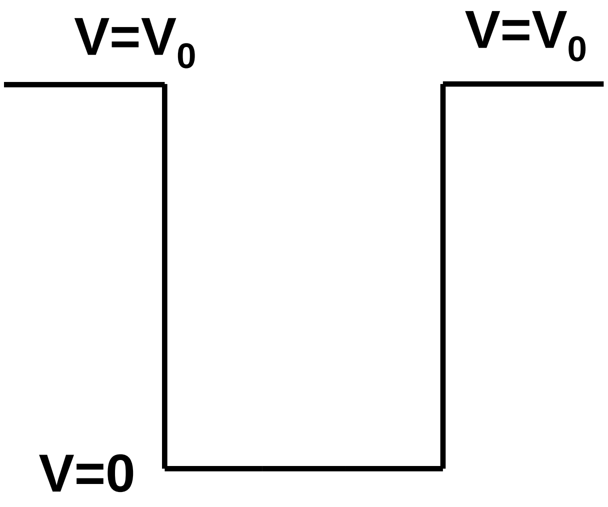
Finite



Question 2:
Can you say which of these two systems has the lowest ground state energy?

A Infinite well
B Finite well
C The same
D No, in the finite well a particle cannot be trapped for ever

Finite



Question 3:
For the finite well, which state has the highest probability for being in a position with V = V_0?

A Eigenstate for E_1
B Eigenstate for E_2
C The same, and probability is non-zero
D Probability is zero (and hence also the same)

Solving eigenfunctions:
General case for time-independent Hamiltonian

Philisophy for various sections with different constant V(x)
Next lecture Harmonic Oscilator => similar for non-constant V(x)

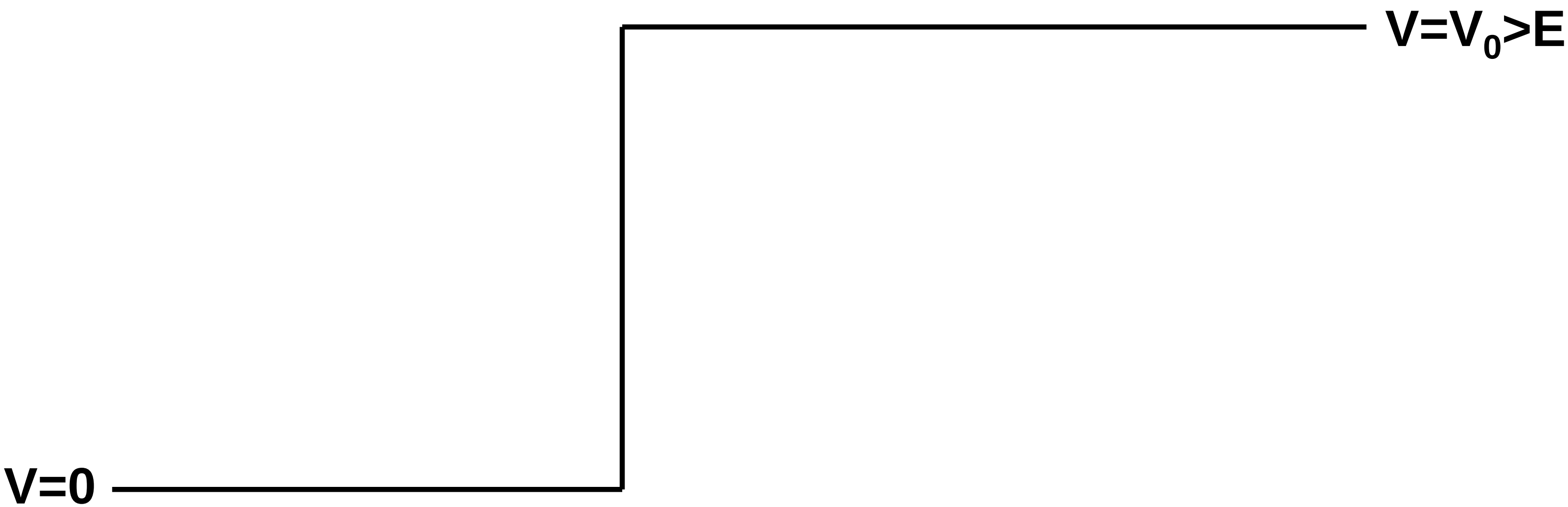
To find Ψ for realistic physical situation, use these boundary conditions (here 1D case):

1. Ψ continuous
2. $d\Psi/dx$ continuous
3. Ψ normalized $\int \Psi^*\Psi \, dx = 1$
4. Ψ limited, no unphysical extremes
5. Ψ is single-valued

(1 and 2:) Otherwise Fourier components with extreme high kinetic energy (high k-values) needed to form Ψ

First the case E < V_0 (details of solution done on blackboard, see also the book)

What is the behavior of a matter wave coming in form the left?



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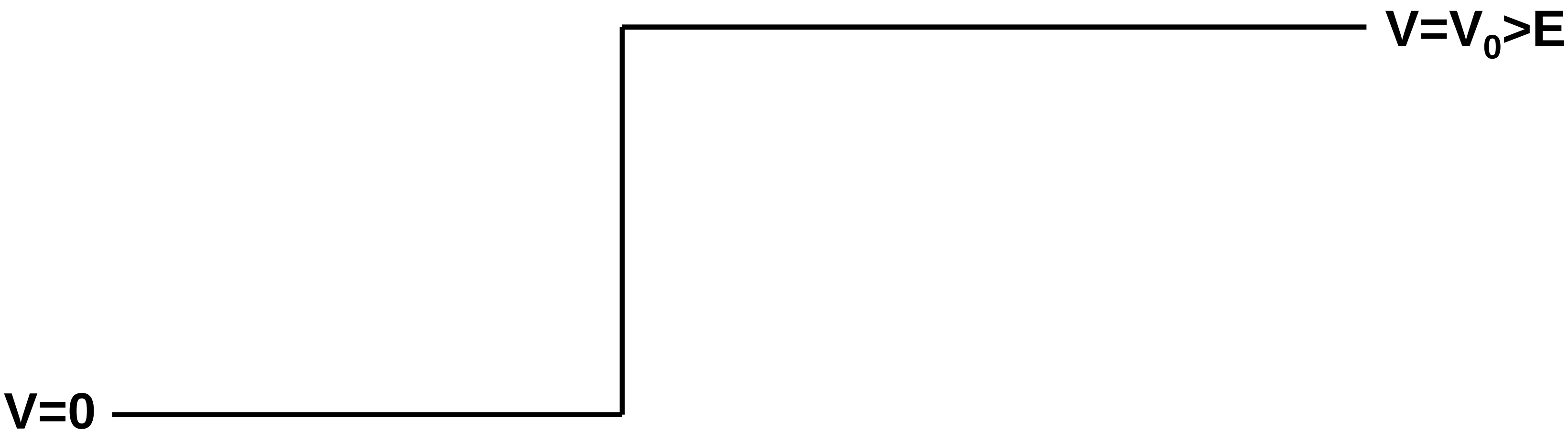
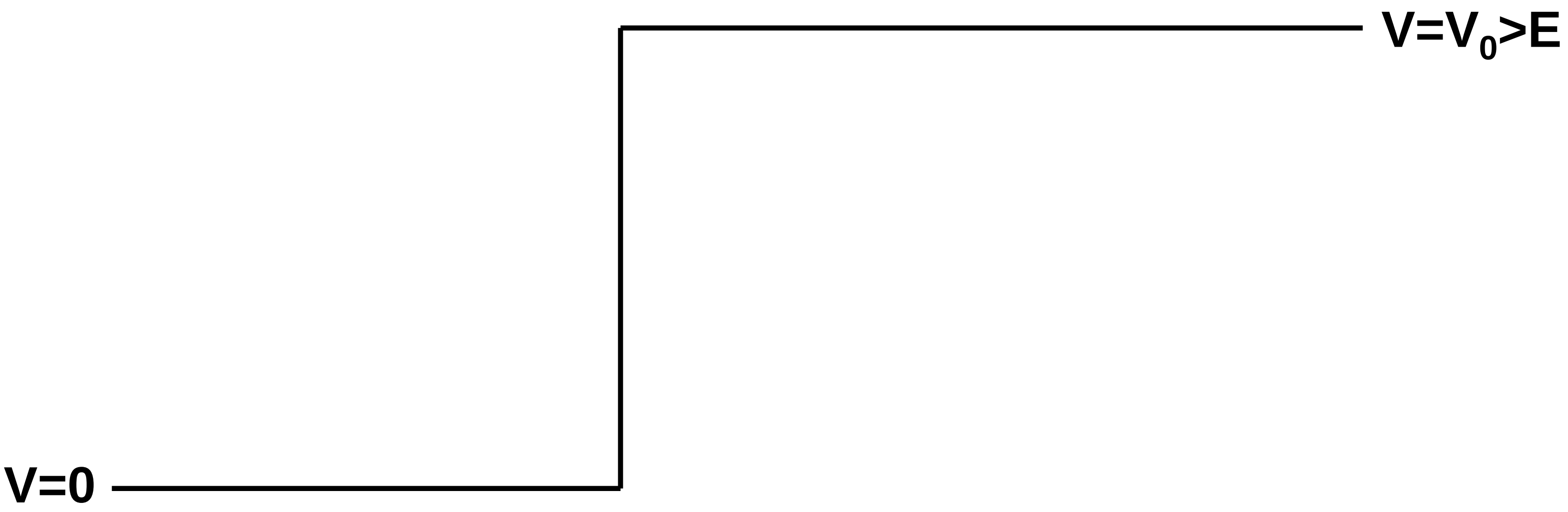


Question 4:

The approach did use states e^{ikx} and not $e^{i(kx-\omega t)}$ and the Time-Ind.Sch.Eq.
How come this can be treated without time dependence?
How come solutions do not show time dependence?

A The analysis is in fact wrong, but a good approximation for during the collision.
B The analysis is right, since the Time-Ind.Sch.Eq. is always valid.
C The analysis is only valid here, since V(x) causes a full reflection.
D The analysis is right, since you can simply add the factor for time dependence $e^{-i\omega t}$ later.

What is the behavior of a matter wave coming in form the left?



Remarks (NOT IN BOOK!):

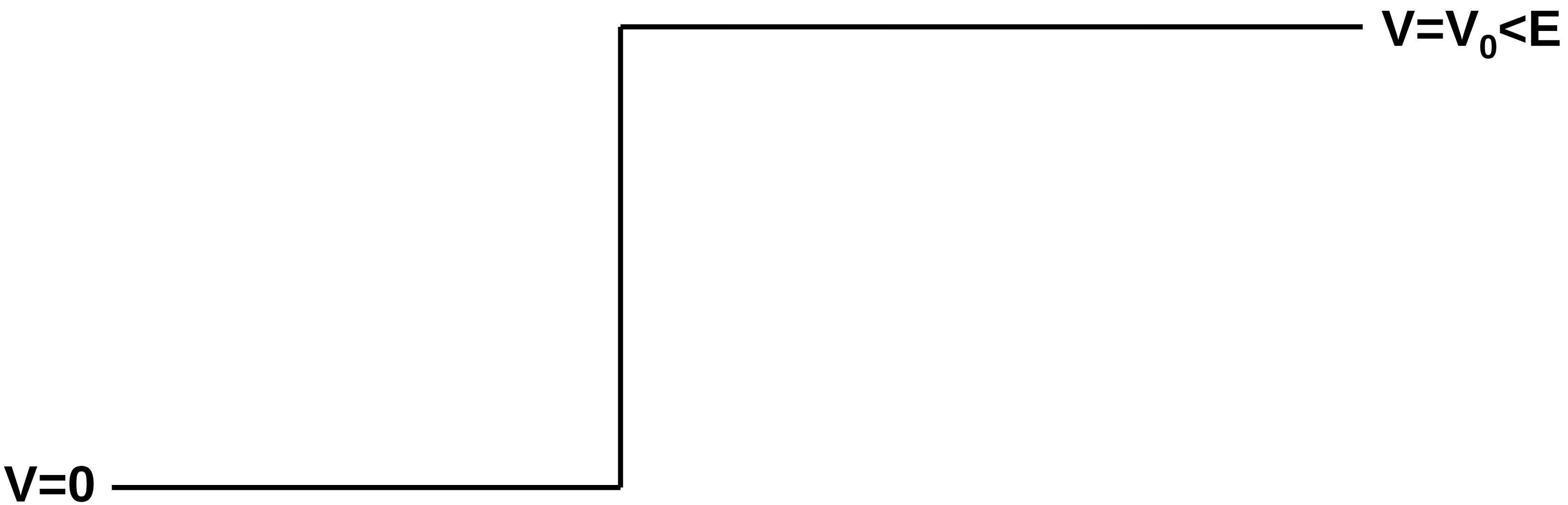
1) The analysis and language used in describing this type of problem is a somewhat loosely defined mixture of a static and a dynamic picture! This can indeed be confusing, but still a widely used model. Think of a snapshot taken, while a very long wave packet is busy with scattering.

2) It is valid for situations where the incoming wave is close to a plane wave. So, it is valid for wave packets that are spread out along x over a long range (Δx large). Such wave packets have small Δp in comparison with <p> (that is, also small quantum uncertainty in the kinetic energy of the particle). The approach is less valid for short wave packets with a large Δp and large quantum uncertainty in kinetic energy.

3) Often they plot Re{e^{ikx}}, etc.

Now the case $E > V_0$

What is the behavior of a matter wave coming in form the left?



Peer instruction question on:

$$T = \left|\frac{C}{A}\right|^2 \frac{k_2}{k_1}$$

$$R = \left|\frac{B}{A}\right|^2$$

$$T + R = 1$$

The part of the wave that gets reflected moves faster than the part that gets transmitted. But keep in mind that the scattering happens in fact with a wave packet. The wave packet that contains the probability spreads out over a smaller range Δx (begin to end fo wave packet) if the velocity is lower.

Why the factor k_2/k_1 ?

A To account for the influence of the wavelength on the transmission and reflection process.

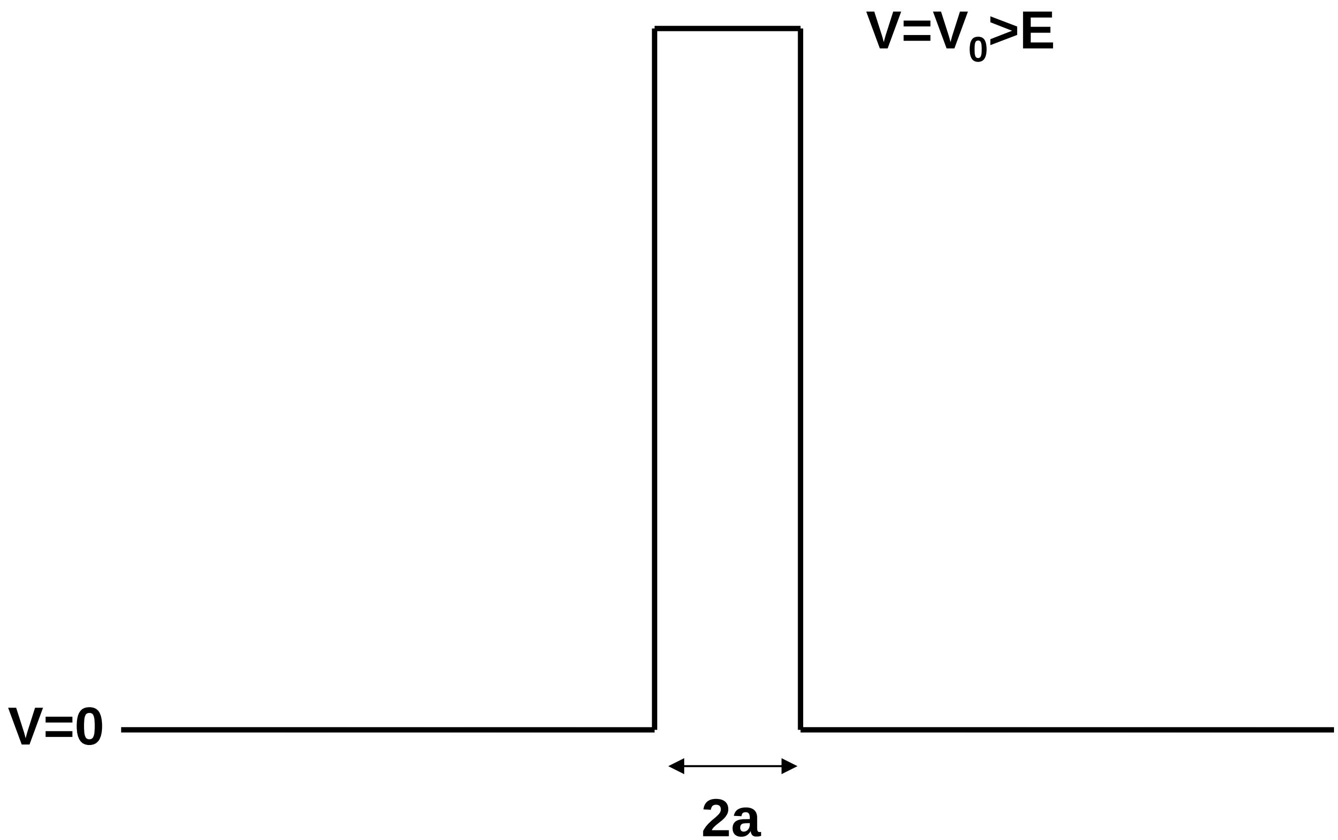
B The probability amplitude C/A has the wrong value, the actual transmitted wave has a higher value because quantum mechanics gives more probability for transmission as compared to classical physics.

C This is in fact wrong, a better calculation will give an answer without the factor k_2/k_1 .

D It accounts for the difference in velocity between the reflected and transmitted particle.

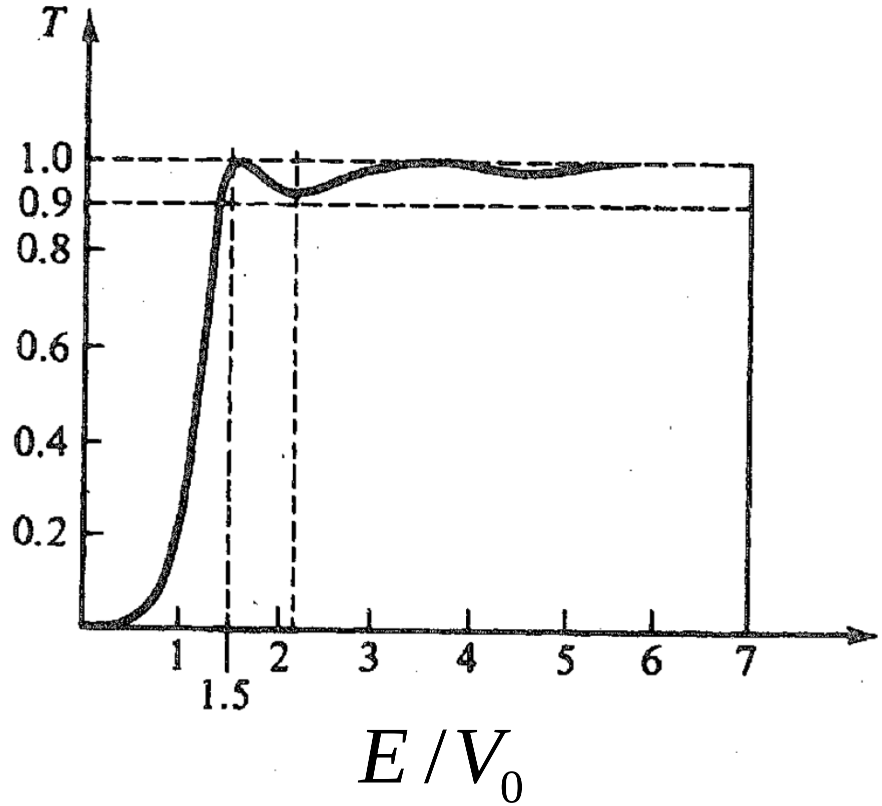
Tunnel effect

What is the behavior of a matter wave coming in form the left?



Griffiths book problem 2.33

See Griffiths book. Eq. [2.169] and problem 2.33



$$T=\frac{1}{1+\frac{1}{4}\frac{V_0^2}{E(V_0-E)}\sinh^2(2k'a)} \quad , \quad E<V_0$$

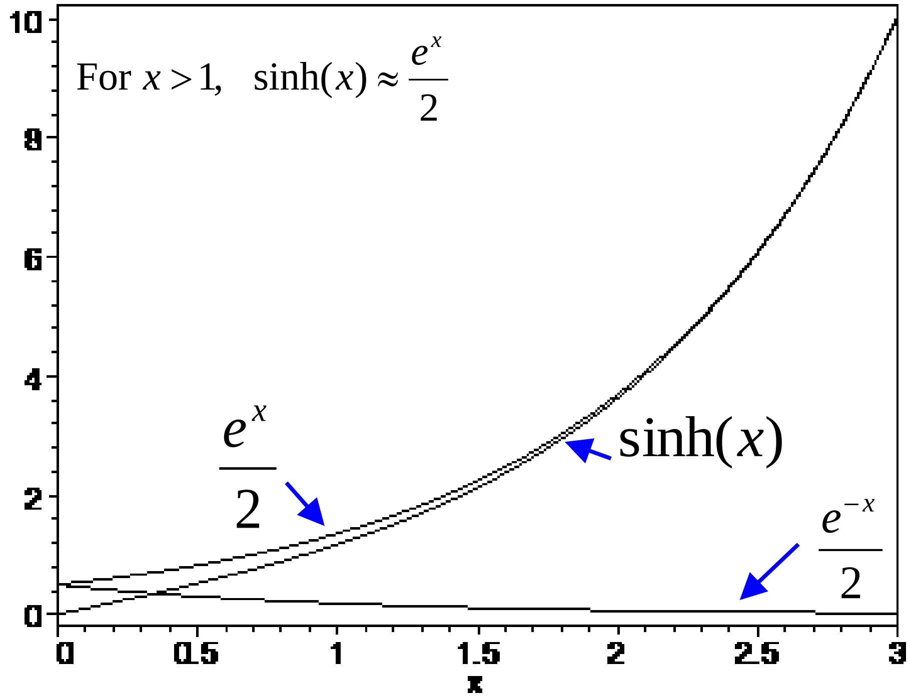
$$T=\frac{1}{1+\frac{1}{4}\frac{V_0^2}{E(E-V_0)}\sin^2(2ka)} \quad , \quad E>V_0$$

$$\sinh x=\frac{e^x-e^{-x}}{2}=\frac{e^{2x}-1}{2e^x}=\frac{1-e^{-2x}}{2e^{-x}}$$

$$k=\sqrt{\frac{2m(E-V_0)}{\hbar^2}}$$ for $E>V_0$ with $e^{\pm ikx}$ solutions

$$k'=\sqrt{\frac{2m(V_0-E)}{\hbar^2}}$$ for $V_0>E$ with $e^{\pm k'x}$ solutions

For a wide range of the parameters, the tunnel transmission (solution for $E<V_0$) goes down exponentially with increasing mass m, and increasing thickness of the barrier a and height of the barrier V_0.



For high and thick tunnel barrier (high *k'a*),

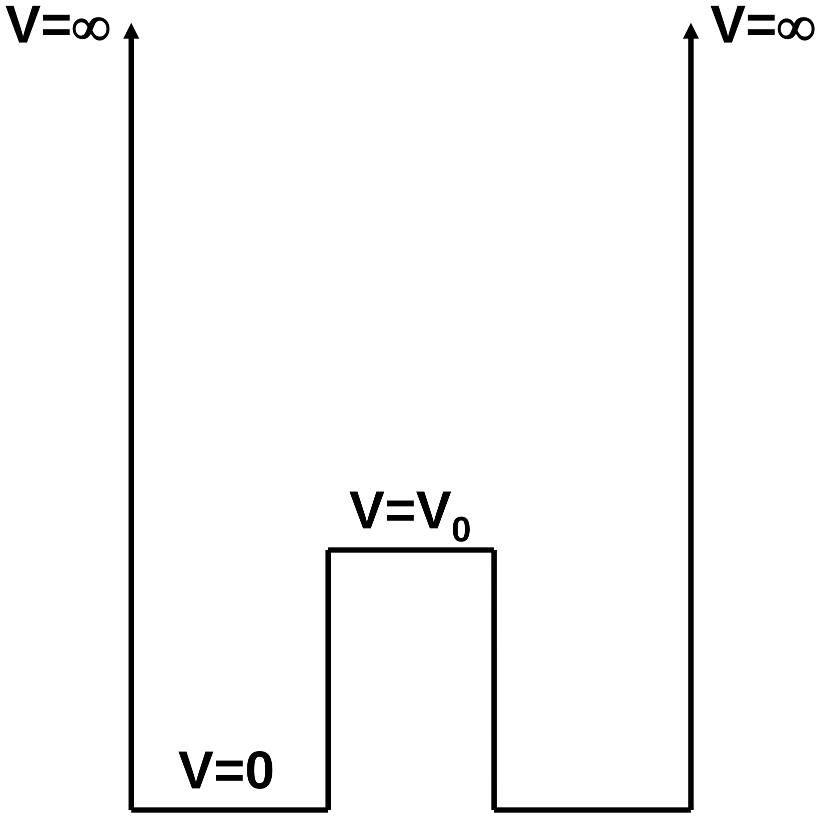
$$T \propto \frac{1}{\sinh^2(2k'a)} \approx 4e^{-4k'a}$$

$$\sinh x = \frac{e^x - e^{-x}}{2} = \frac{e^{2x}-1}{2e^x} = \frac{1-e^{-2x}}{2e^{-x}}$$

Coupling 2 quantum systems: LCAO

Linear Combination of Atomic Orbitals

Weakly couple two quantum wells, with a single particle in the total system. What is the new wave function for the ground state?



Next slides show the approach as in problem W4.1 where we directly calculate the new energy eigenstates and eigenvalues of the system if the two wells are coupled, by solving the time-independent Schrödinger equation as a 2 by 2 matrix.

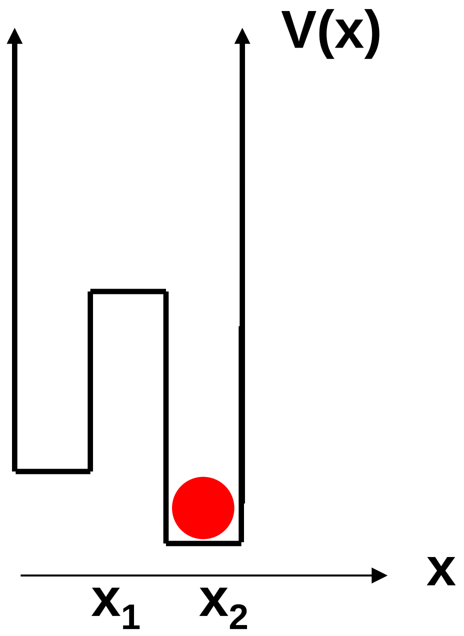
Two coupled wells $\hat{H} = \hat{H}_E + \hat{H}_T \leftrightarrow \begin{pmatrix} E_1 & T \\ T & E_2 \end{pmatrix} = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix} + \begin{pmatrix} 0 & T \\ T & 0 \end{pmatrix}$

Tunnel coupling gives OFF-DIAGONAL ELEMENTS

E_i describes the energy of the system when it is only in the well at x_i

T describes the energy associated with the mechanism that makes transitions from well 1 to well 2, and vice versa, possible.

Mechanical system, with 2 states



See also problem W4.1

Assume $E_2 = E_1$

$$\hat{H} = \hat{H}_E + \hat{H}_T \leftrightarrow \begin{pmatrix} E_1 & T \\ T & E_1 \end{pmatrix} = \begin{pmatrix} E_1 & 0 \\ 0 & E_1 \end{pmatrix} + \begin{pmatrix} 0 & T \\ T & 0 \end{pmatrix}$$

$$\begin{pmatrix} E_1 & T \\ T & E_1 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}_i = E_i \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}_i \quad \Rightarrow$$

New eigenvalues E_g and E_e

(Note that this equation is the time-indepent Schrödinger equation)

Fill in for the general solution for 2x2 eigenvalue problem:

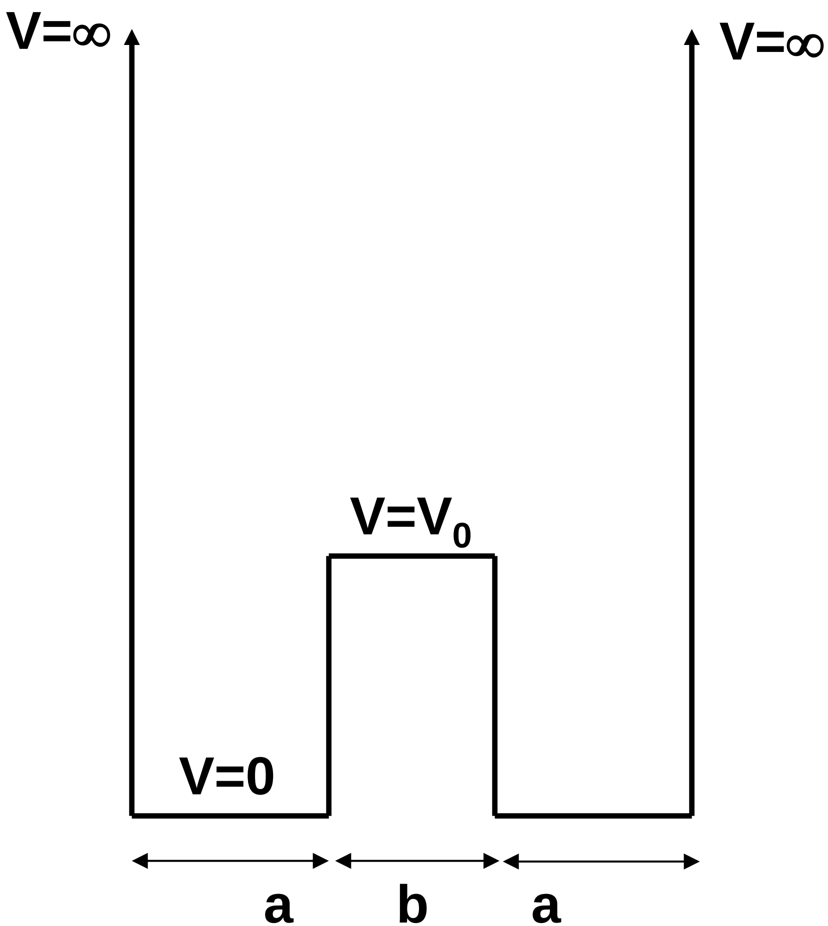
$$\begin{cases} E_g = \dfrac{E_1 + E_1}{2} - \dfrac{1}{2}\sqrt{(E_1 - E_1)^2 + 4T^2} = E_1 + T = E_1 - |T| \\ E_e = \dfrac{E_1 + E_1}{2} + \dfrac{1}{2}\sqrt{(E_1 - E_1)^2 + 4T^2} = E_1 - T = E_1 + |T| \end{cases}$$

$$(\text{the choice of } + \text{and} - \text{here assumes } T < 0)$$

See also problem W4.1

What is the wavefunction for the ground state?

The symmetric or the anti-symmetric superposition?

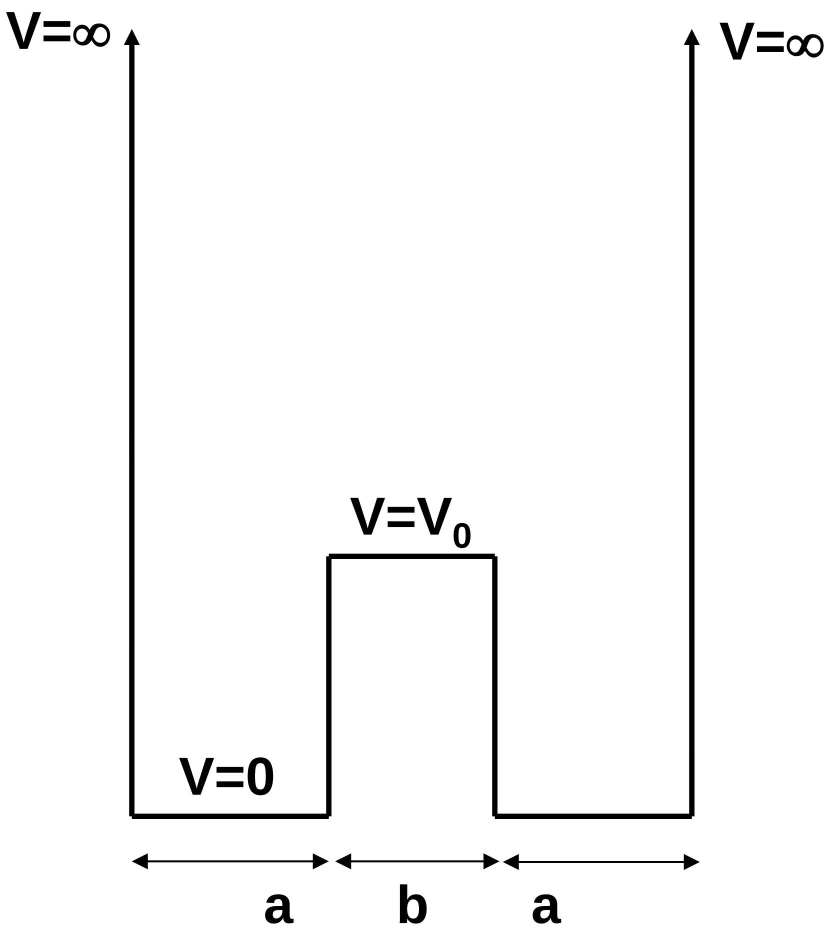


See also problem W4.1

For the lowest two energy eigenstates:

Write down an expression for calculating the amount of potential energy and kinetic energy that are present in E_g and E_e.

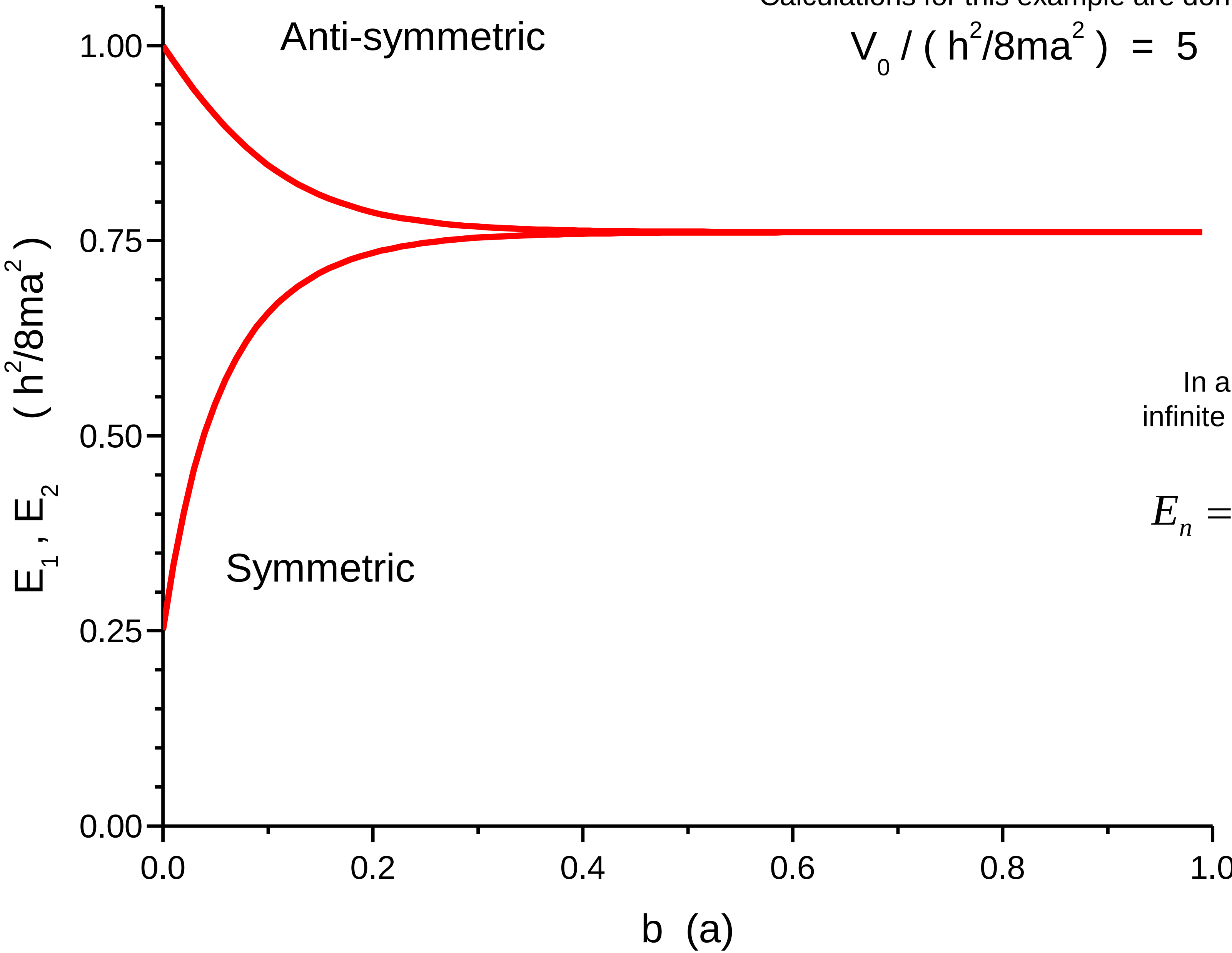
Choose wise whether to do it in x-representation or k-representation.



See also problem W4.1

Calculations for this example are done for

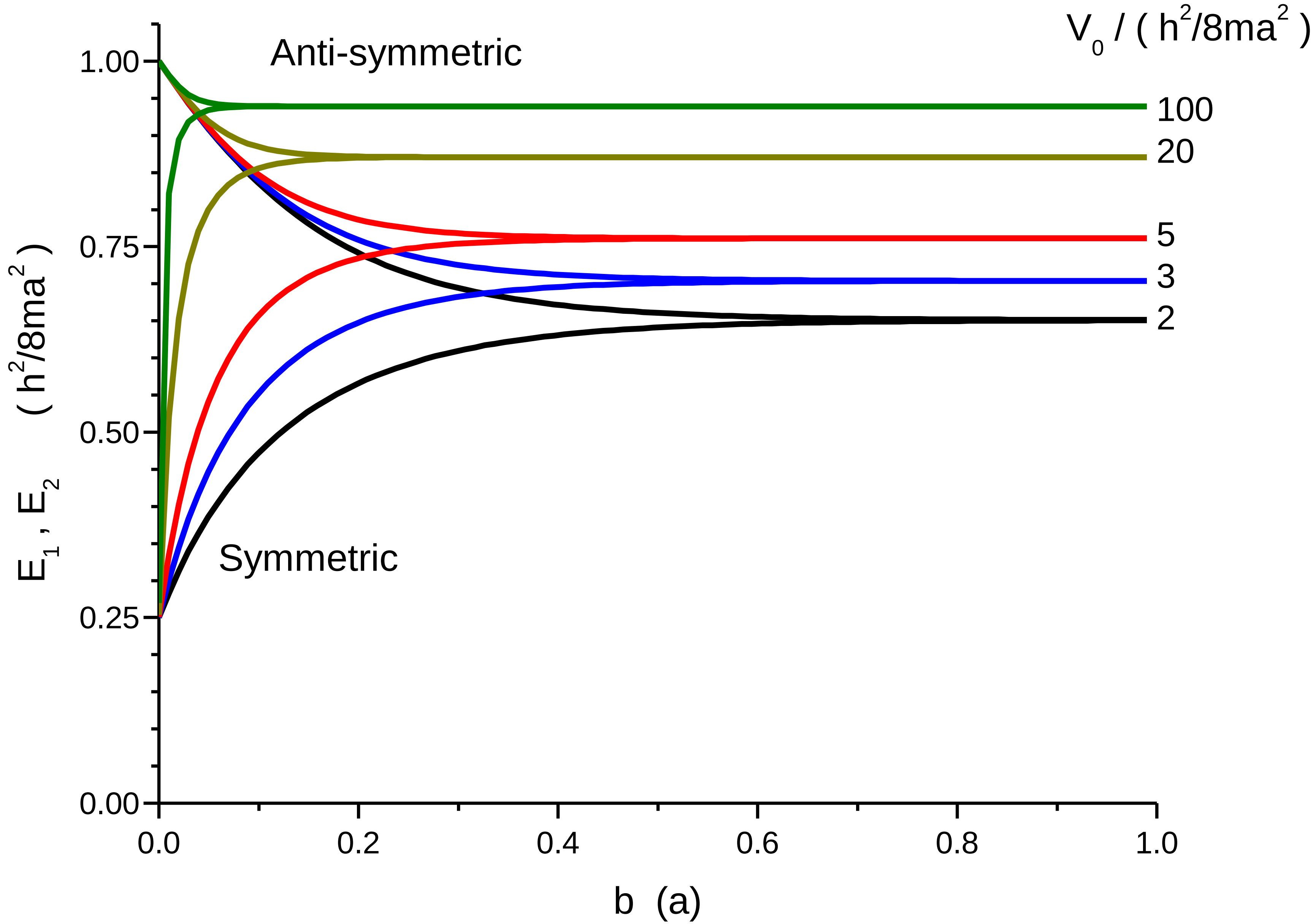
$V_0 / (h^2/8ma^2) = 5$



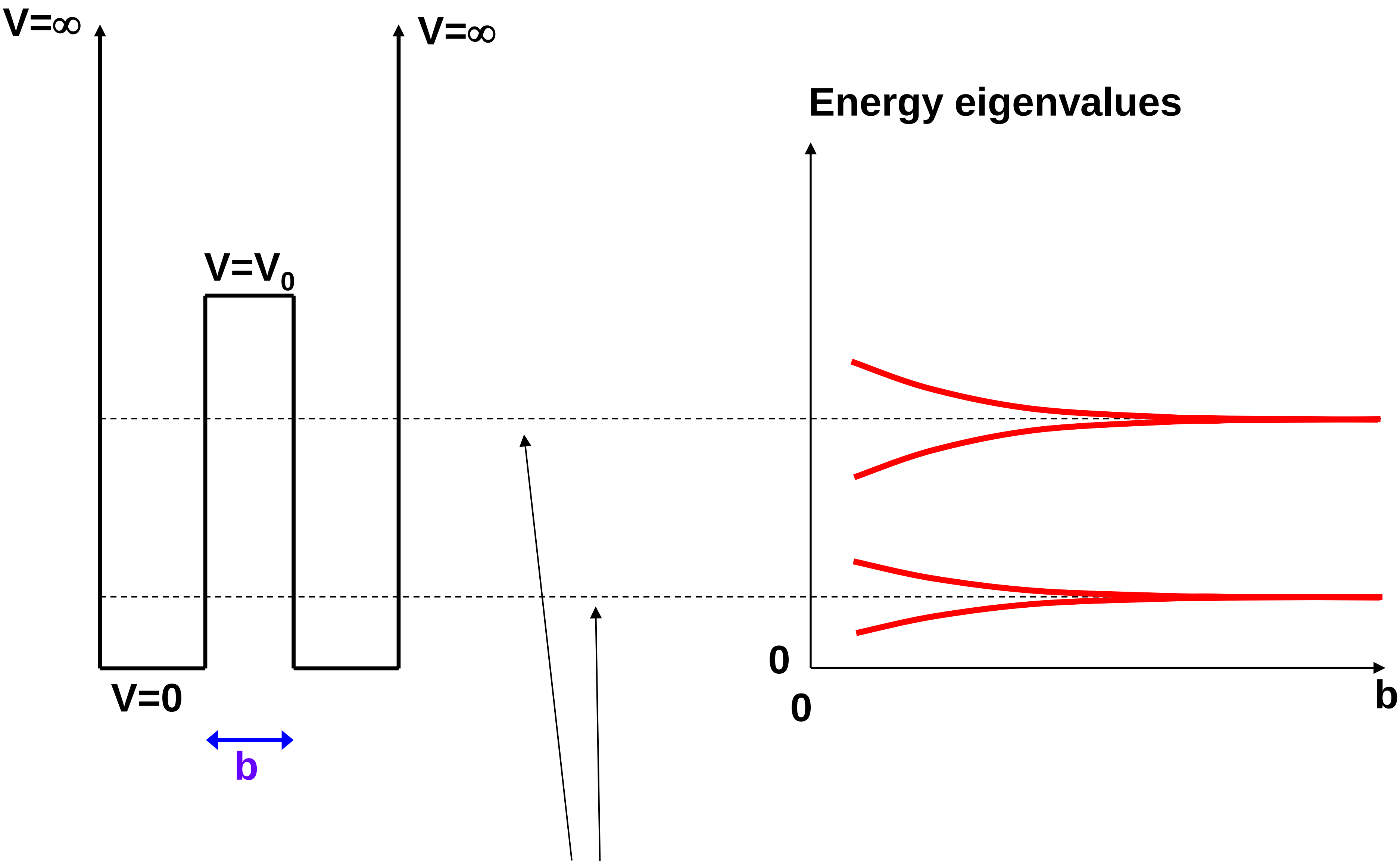
In a single infinite deep well

$$E_n = \frac{n^2 h^2}{8ma^2}$$

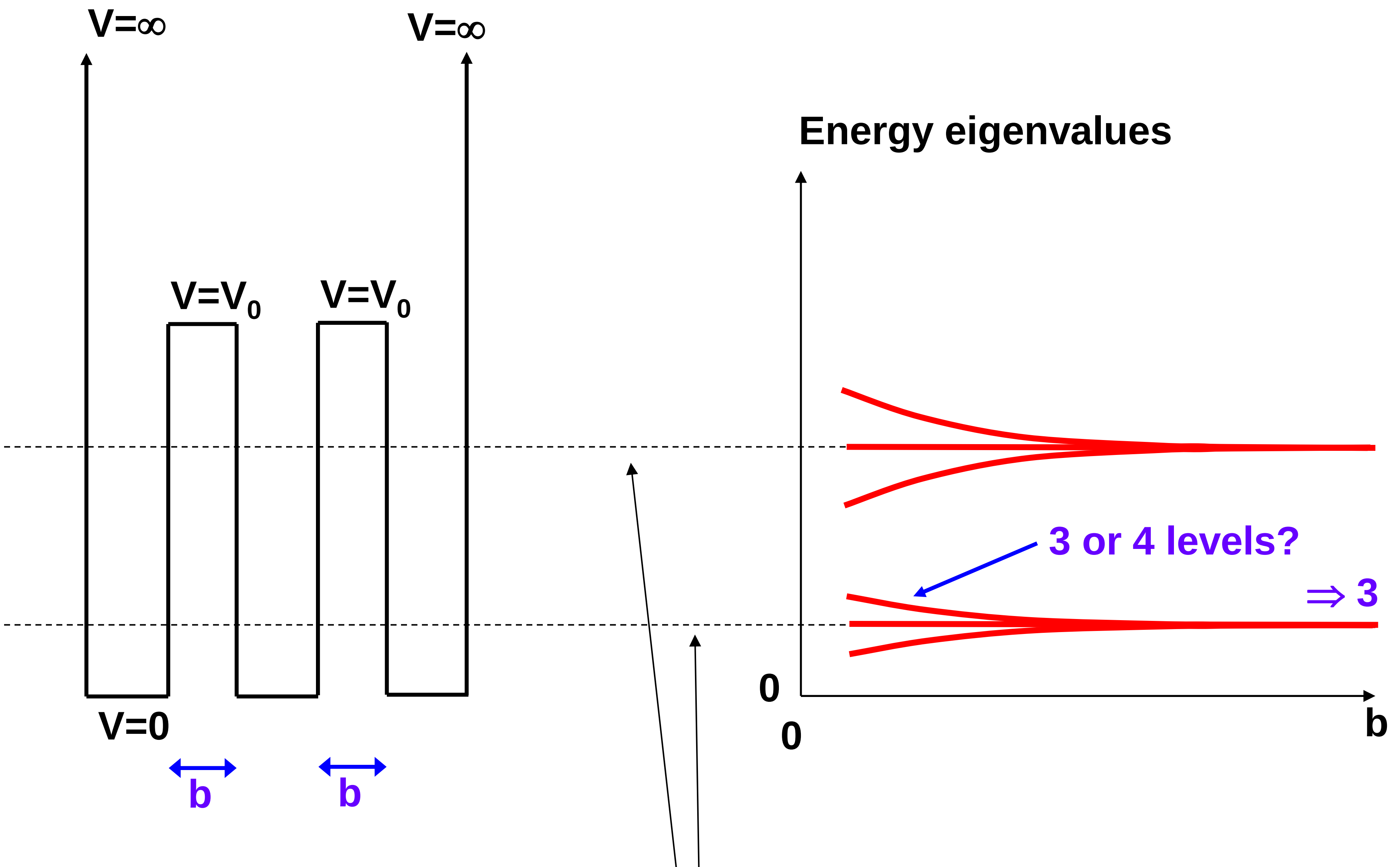
See also problem W4.1



Anti-symmetric
Symmetric
V_0 / ($h^2/8ma^2$)
100
20
5
3
2
E_1 , E_2 ($h^2/8ma^2$)
1.00
0.75
0.50
0.25
0.00
0.0
0.2
0.4
0.6
0.8
1.0
b (a)



Energy levels for isolated potential wells



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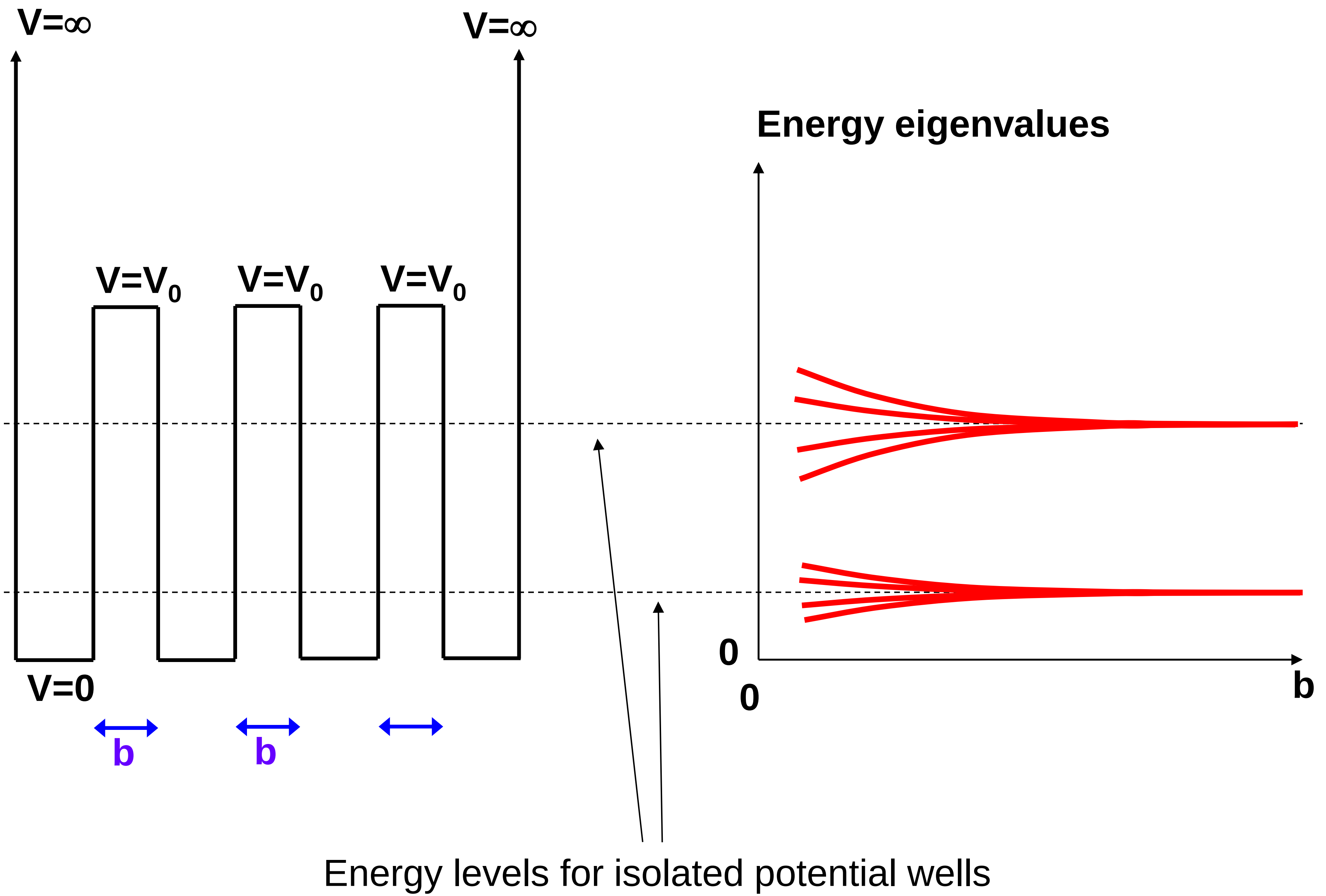
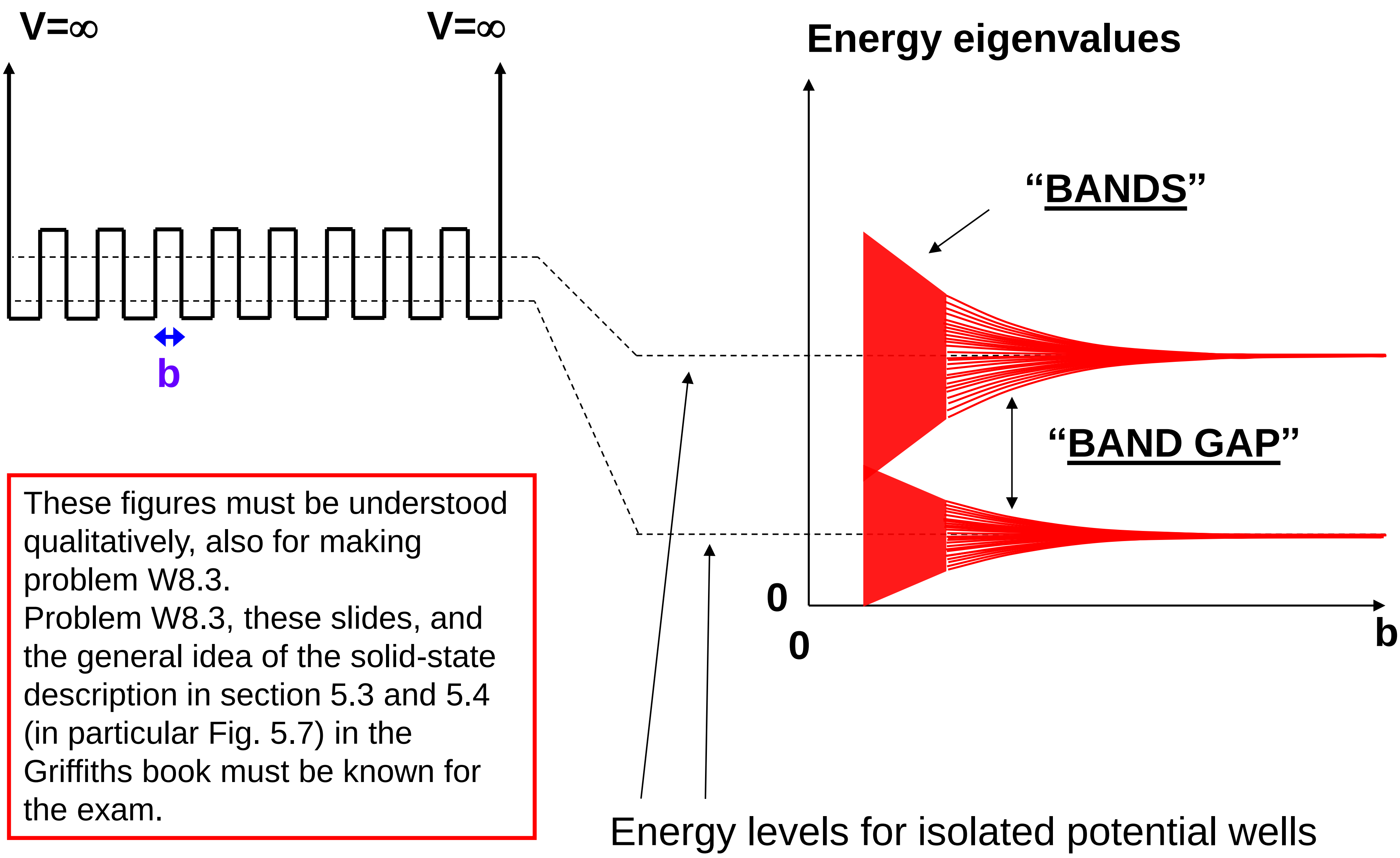


V=∞
V=∞
V=V0
V=V0
V=V0
V=0
b
b
Energy eigenvalues
0
0
b
Energy levels for isolated potential wells

From 1D potential well to solid state material



These figures must be understood qualitatively, also for making problem W8.3.
Problem W8.3, these slides, and the general idea of the solid-state description in section 5.3 and 5.4 (in particular Fig. 5.7) in the Griffiths book must be known for the exam.

Why is gold a conductor, and glass not?

Why are some materials transparent?

What is electrical current in a metal?

(worked out on the blackboard)

Summary:

1. Wavefunction incident on finite potential

2. Tunnel effect

3. Solid state physics has its basis in the physics of a particle in a quantum well (particle in a box)