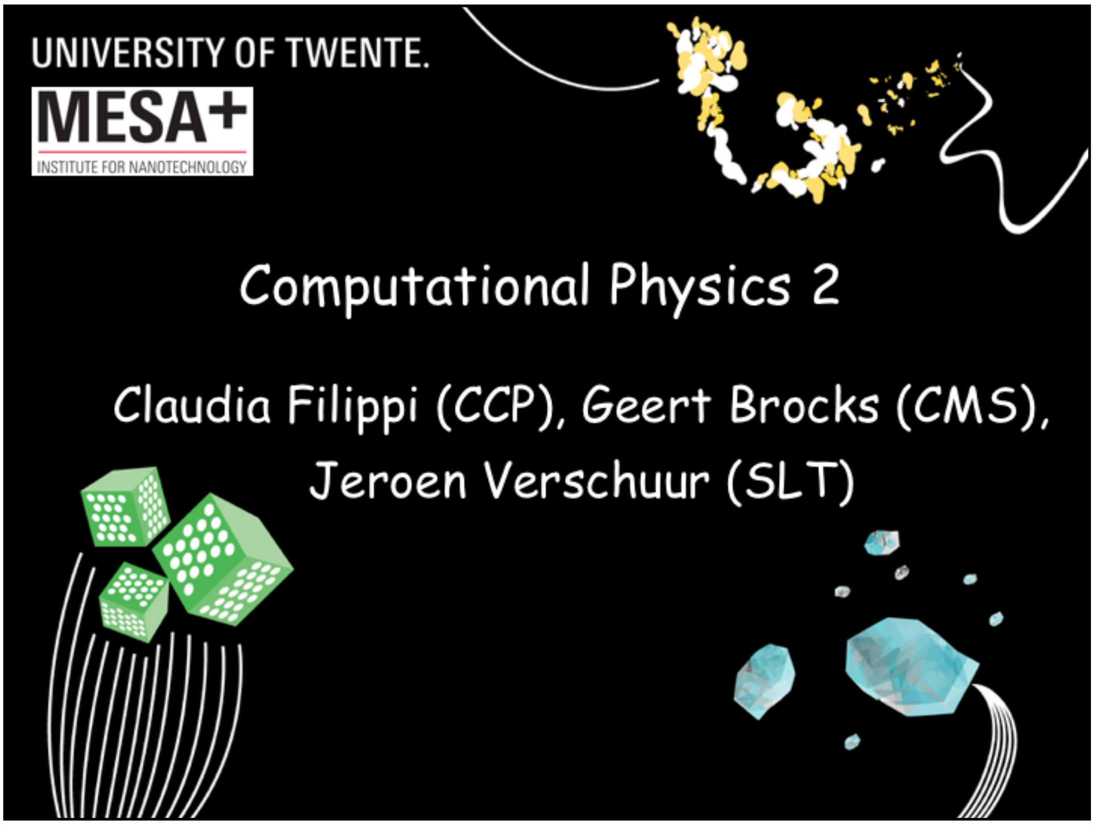
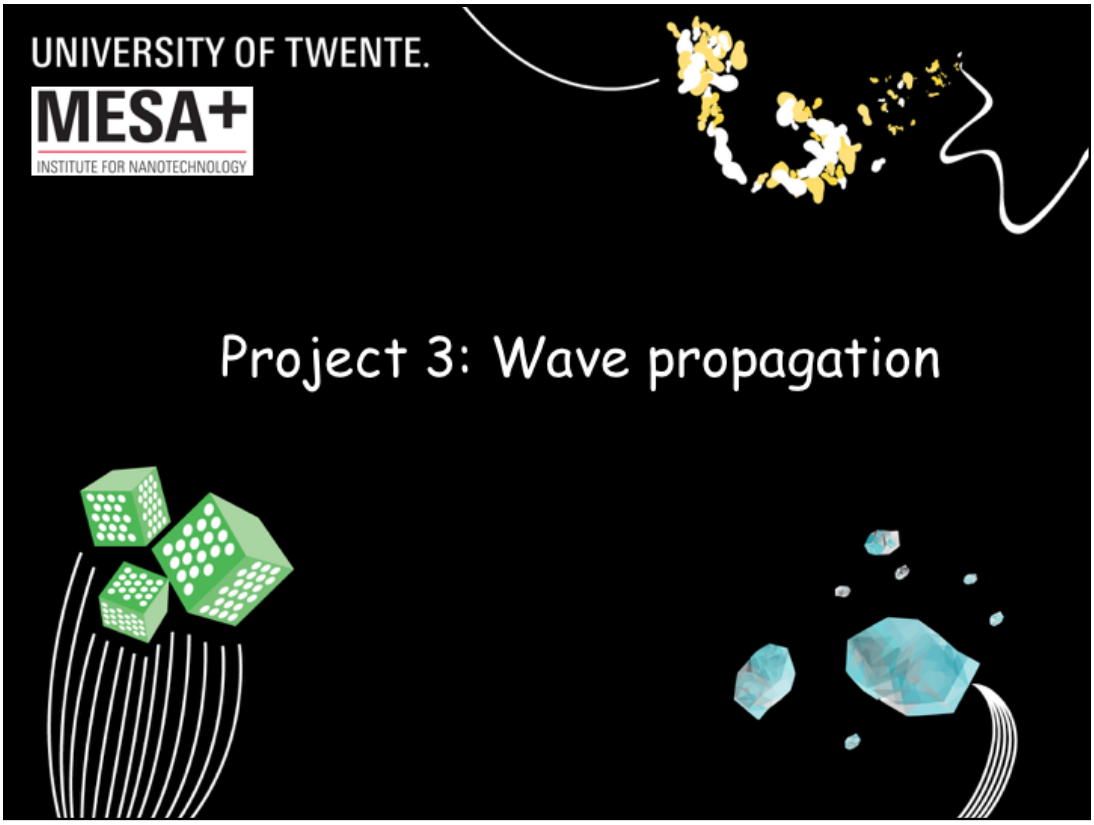
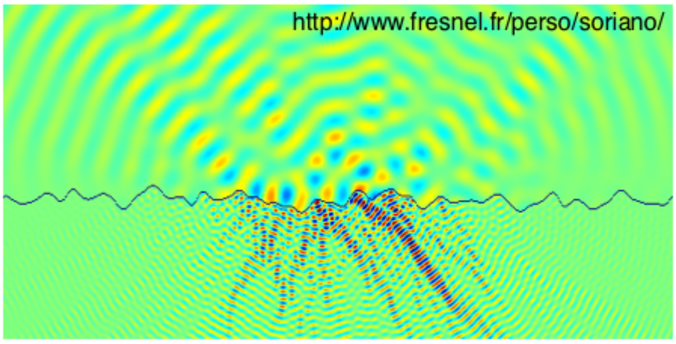


The set-up of computational physics 2 is the same as of computational physics 1.



The first project is about propagation of waves.

Project 3: wave propagation $\mathbf{M} = \mathbf{M}(x_1)\mathbf{M}(x_2)\ldots\mathbf{M}(x_n)$



$$\nabla^2 P(\mathbf{r},t) = \frac{1}{v_s^2}\frac{\partial^2 P(\mathbf{r},t)}{\partial t^2}$$ acoustic waves

$$\nabla^2 \vec{E}(\mathbf{r},t) = \epsilon\,\mu\,\frac{\partial^2 \vec{E}(\mathbf{r},t)}{\partial t^2}$$ electromagnetic waves

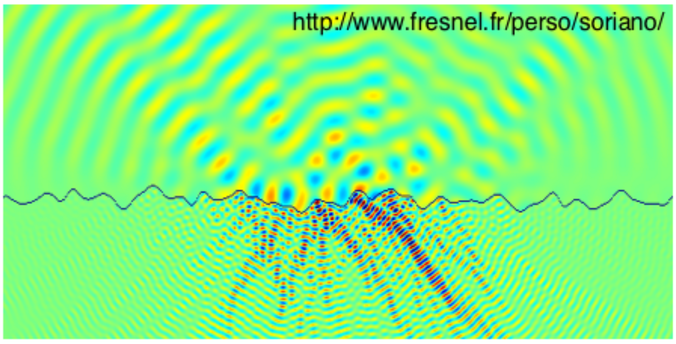
$$\boxed{-\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r},t) + V(\mathbf{r})\Psi(\mathbf{r},t) = i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t}}$$ quantum waves

Waves are the solution of a wave equation:

- the "simplest" wave equation is the one for acoustic waves, where $P(\mathrm{r},\boldsymbol{t})$ is the pressure as a function of position and time, and v_S is the sound velocity
- you all know the wave equation for electromagnetic waves. Here only the part for the electric field $\vec{E}(\mathrm{r},\boldsymbol{t})$, where $v = 1/\sqrt{\epsilon\mu}$ is the speed of light in the medium.
- although looking a bit different from the previous two, the Schrodinger equation is also a wave equation. It describes the propagation of electron waves, for instance.

This project concerns electron waves only (it has to fit within a couple of weeks), but the numerical approaches used, are also suitable to describe the propagation of sother waves, such as electromagnetic or acoustic ones.

Stationary quantum waves



$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r},t) + V(\mathbf{r})\Psi(\mathbf{r},t) = i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t}$$ quantum waves

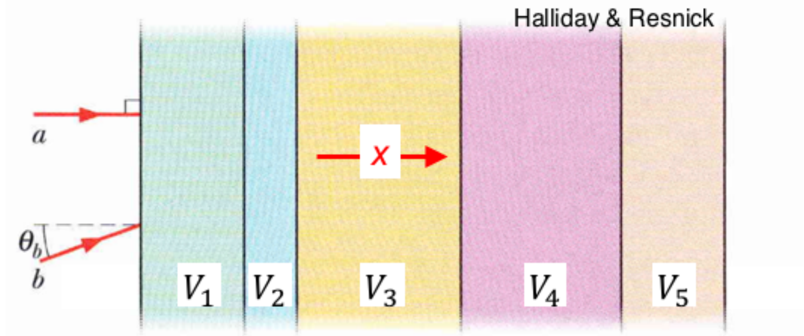
$$\Psi(\mathbf{r},t) = \psi(\mathbf{r})\exp[-i\omega t]$$ stationary waves

$$\boxed{-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r})} \qquad E = \hbar\omega$$

So we restict ourselves to quantum waves in the following. We will also restrict ourselves to stationary waves, which, per definition, can be written as $\Psi(\mathbf{r},t) = \psi(\mathbf{r};\omega)\exp[-i\omega t]$ with $\omega = E/\hbar$. This is not a giant restriction, because you know from Fourier transform theory that, if you have the solution for any frequency ω, then any solution of the wave equation can be constructed as a sum of different frequencies $\Phi(\mathbf{r},t) = \int_{-\infty}^{\infty} a(\omega)\,\psi(\mathbf{r};\omega)\exp[-i\omega t]\,d\omega$. The functions $\psi(\mathbf{r};\omega)$ are the solutions of the time-independent Schrodinger equation $-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r})$. This is what we will do in the following.

Stationary quantum waves in layered media

$V(\mathbf{r}) =$

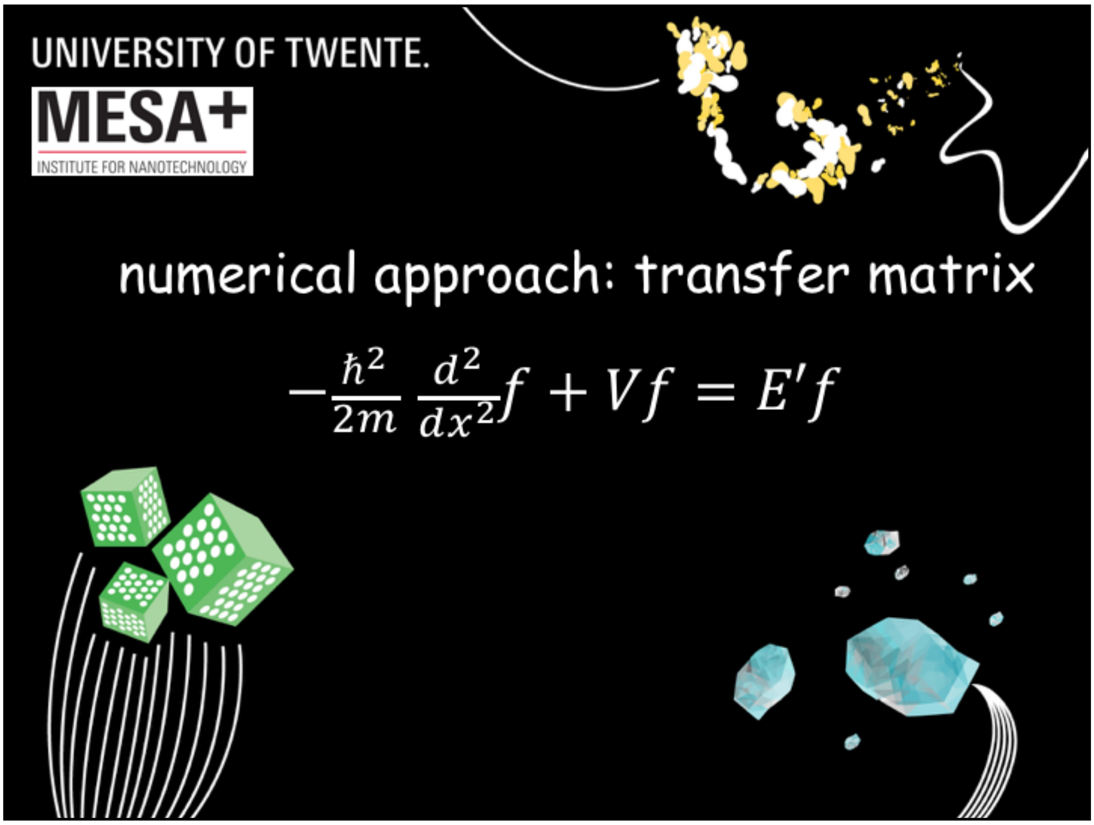


$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r})$$ stationary waves

$$V(\mathbf{r}) = V(x) \qquad \psi(\mathbf{r}) = f(x)\exp[ik_y y + ik_z z]$$ layered media

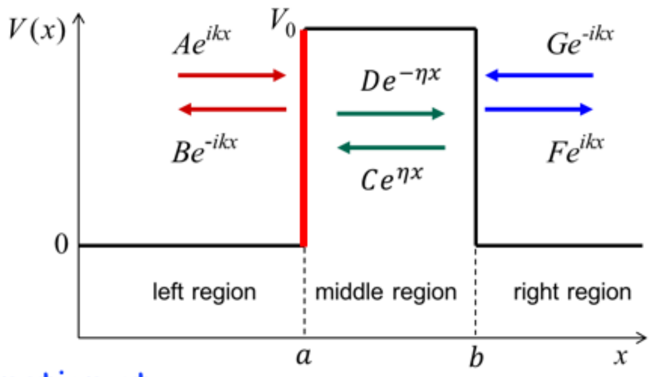
$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}f(x) + V(x)f(x) = E'f(x)} \qquad E' = E - \frac{\hbar^2}{2m}[k_y^2 + k_z^2]$$

To limit the computational requirements, we will limit ourselves to special potentials $V(\mathbf{r}) = V(x)$, which describes layered media (a somewhat specialized, but technically important application). Using separation of variables, one can immediately write down the solutions for the y- and z-dependencies of the function: plane waves $\exp[ik_y y]$ and $\exp[ik_z z]$. Using this in the Schrodinger equation then gives an effective one-dimensional Schrodinger equation for the unknown factor $f(x)$.



Given this one-dimensional Schrodinger equation, we wish to solve it to describe propagation of waves. We are going to use a technique called the transfer matrix algorithm.

Elementary quantum mechanics: the square barrier



wave function at $x = a$

continuous $\quad Ae^{ika} + Be^{-ika} = Ce^{\eta a} + De^{-\eta a}$

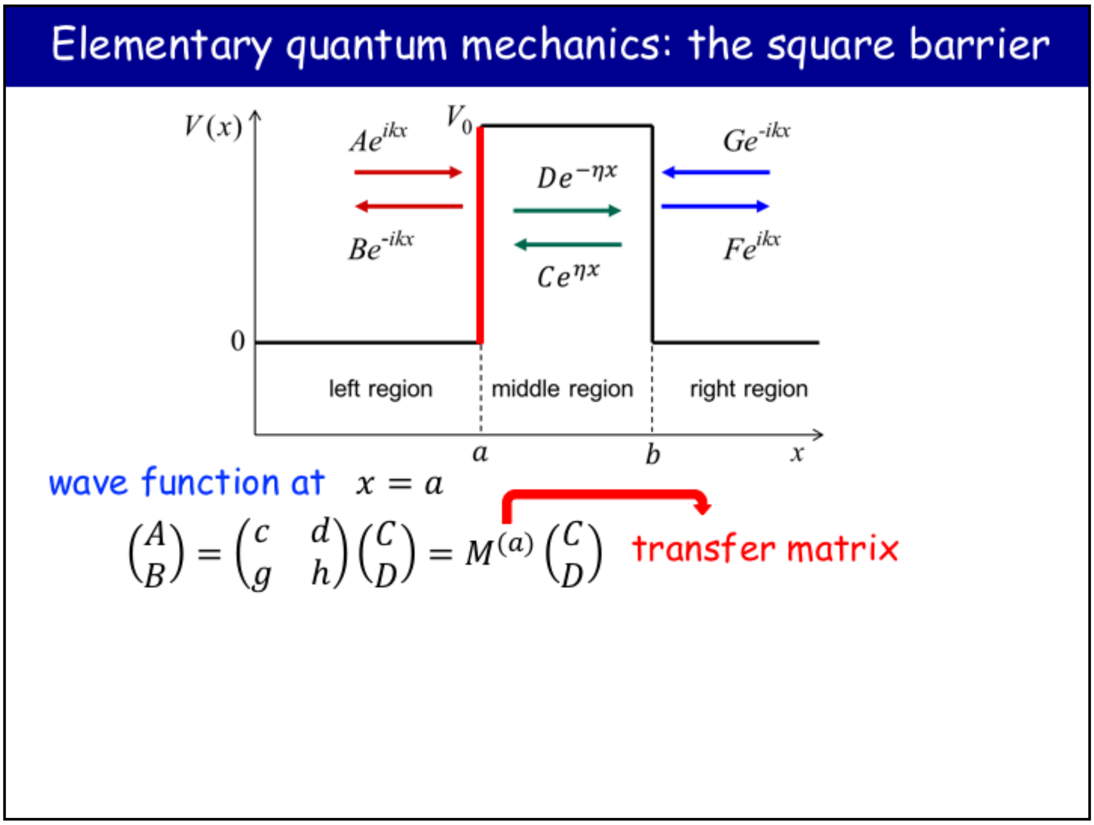
differentiable $\quad ikAe^{ika} - ikBe^{-ika} = \eta Ce^{\eta a} - \eta De^{-\eta a}$

in matrix form: $\quad \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} c & d \\ g & h \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix}$

Start with a simple, textbook example: the square barrier. In the most general set-up, we have a wave $A\exp[ikx]$ coming in from the left, and a wave $G\exp[-ikx]$ coming in from the right, where $k = \sqrt{2mE}/\hbar$. In the barrier we have evanescent waves $C\exp[\eta x]$ and $D\exp[-\eta x]$, with $\eta = \sqrt{2m(V_0 - E)}/\hbar$. The waves $B\exp[-ikx]$ and $F\exp[ikx]$ describe the reflected and the transmitted waves, propagating to the right and to the left respectively. [To assess the propagation direction, one has to remember the time-dependent part $\exp[-i\omega t]$, which, for instance, gives $A\exp[i(kx - \omega t)]$; this clearly is a wave propagating to the right.]

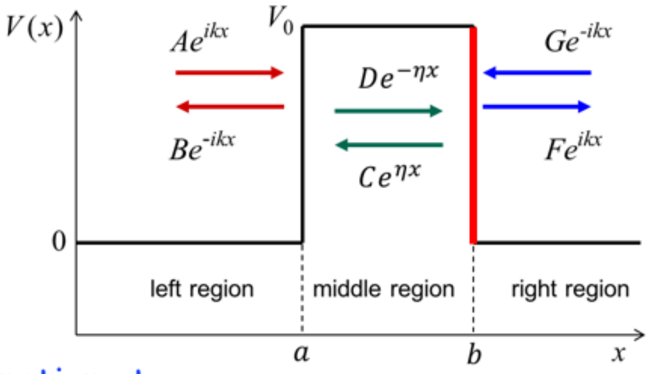
We know the functional form of the solutions in the individual regions. We may know the amplitudes of the incoming waves A and G (because we send in the waves ourselves), but we do not yet know the amplitudes $B, C, D,$ and F. Elementary quantum mechanics tells you that, if we connect the function pieces that are solutions in the different regions, to one complete function that is continuous and differentiable, then we have found a solution to the Schrodinger equation (which is the solution, as there is no other one, given these boundary conditions.

Let us start with the left potential step and write down the conditions for continuity and differentiability (the first derivative being continuous). These conditions can be rewritten in matrix-vector form, connecting the amplitudes A, B left of the step to C, D right of the step. The connecting matrix coefficients a,b,c,d you can figure our yourselves (ot have a look at the lecture notes, section 1).



The matrix $M^{(a)}$ connecting the amplitudes right to left of the potential step is called the *transfer matrix*.

Elementary quantum mechanics: the square barrier



wave function at $x = a$

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} c & d \\ g & h \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} = M^{(a)} \begin{pmatrix} C \\ D \end{pmatrix}$$ transfer matrix

wave function at $x = b$

$$\begin{pmatrix} C \\ D \end{pmatrix} = \begin{pmatrix} c' & d' \\ g' & h' \end{pmatrix} \begin{pmatrix} F \\ G \end{pmatrix} = M^{(b)} \begin{pmatrix} F \\ G \end{pmatrix}$$

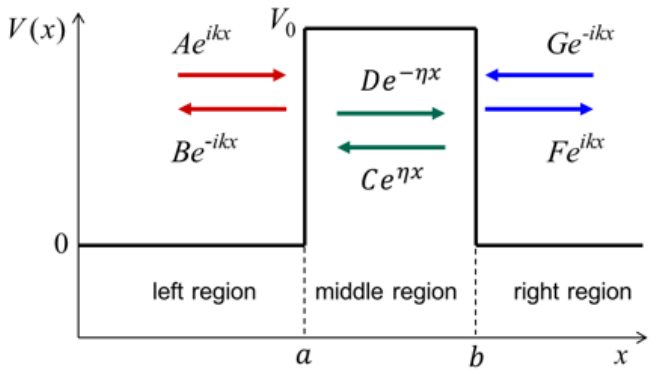
relating amplitudes

$$\begin{pmatrix} A \\ B \end{pmatrix} = M^{(a)} M^{(b)} \begin{pmatrix} F \\ G \end{pmatrix}$$

One can of course do the same trick (wave function continuous and differentiable) at the right potential step ($x = b$), connecting the amplitudes F, G to C, D via de transfer matrix $M^{(b)}$.

This now allows one to connect the amplitudes A,B left of the barrier to those right of the barrier F,G. The transfer matrix $M = M^{(a)} M^{(b)}$ doing the connection throught the barrier is simply the matrix product of the transfer matrices of the two individual steps.

Elementary quantum mechanics: the square barrier



relating amplitudes with transfer matrix

$$\begin{pmatrix} A \\ B \end{pmatrix} = M^{(a)} M^{(b)} \begin{pmatrix} F \\ G \end{pmatrix} \equiv M \begin{pmatrix} F \\ G \end{pmatrix}$$

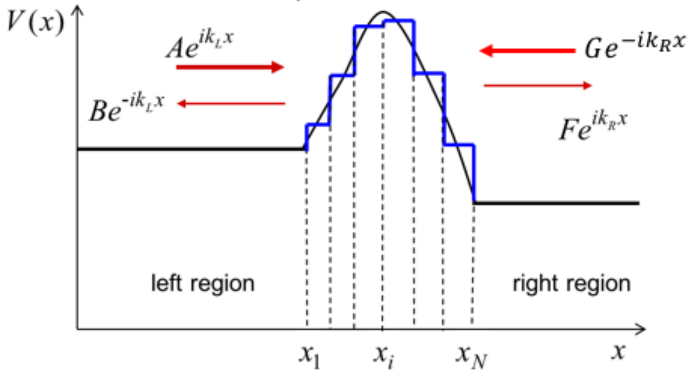
$$T = \frac{|F|^2}{|A|^2} = \frac{1}{|M_{11}|^2} \qquad R = \frac{|B|^2}{|A|^2} = \frac{|M_{21}|^2}{|M_{11}|^2}$$

transmission coefficient   reflection coefficient

In principle the problem is now solved. We know the amplitudes A, G on forehand (they are incoming waves, so their amplitude is set by the experimenter), and we can determine the amplitudes B, F by solving this linear equation (by the way, this method for looking at tunneling through a square barrier, is a lot easier than the one that is ususally applied in textbooks, such as Grffiths).

The usual experimental set-up has $G = 0$, i.e., no waves coming in from the right. Then T is called the transmission coefficient, and describes the tunneling probability through the barrier, whereas R is the reflection coefficient.

Transfer matrix algorithm, barrier of any shape



relating amplitudes with transfer matrix

$$\begin{pmatrix} A \\ B \end{pmatrix} = M^{(1)} M^{(2)} \ldots M^{(N-1)} M^{(N)} \begin{pmatrix} F \\ G \end{pmatrix} \equiv M \begin{pmatrix} F \\ G \end{pmatrix}$$

$$T = \frac{v_L |F|^2}{v_R |A|^2} = \frac{v_L}{v_R} \frac{1}{|M_{11}|^2}$$ transmission coefficient

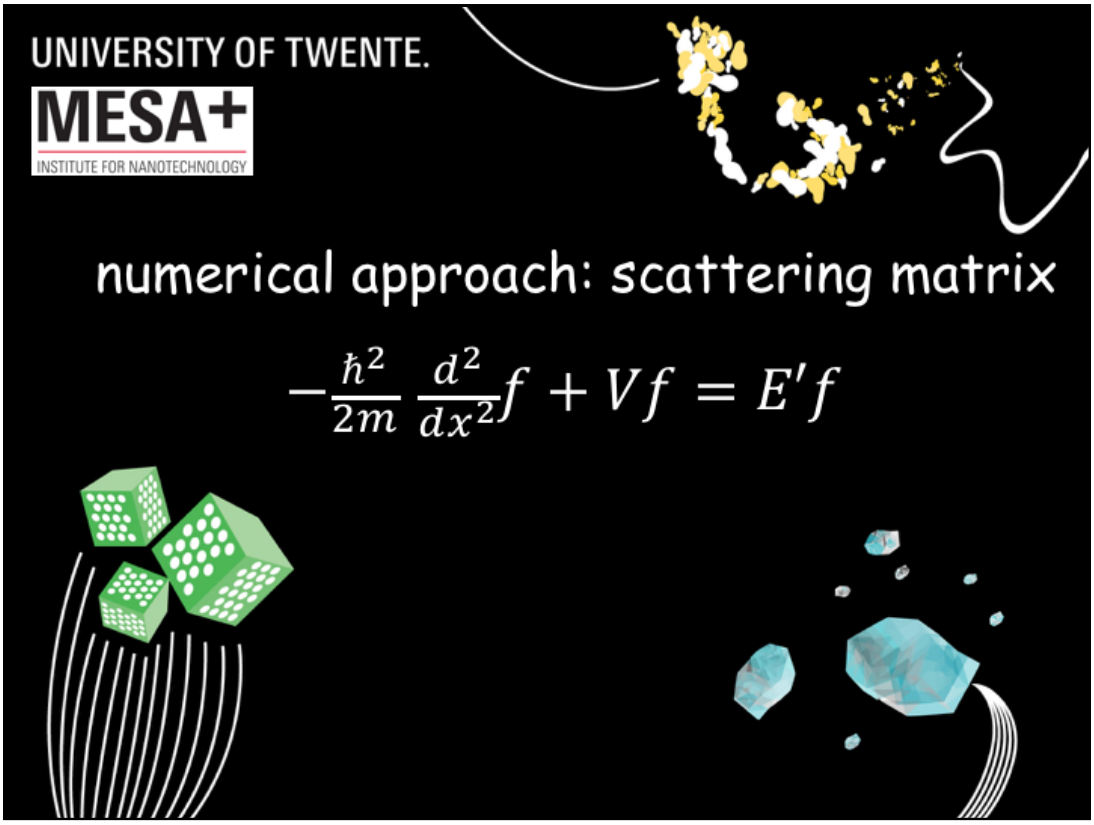
The transfer matrix approach is very general, and can be used to describe reflection/transmission of a barrier of any shape, or indeed of a potential well instead of a barrier, or any combination of wells and barriers.

Simply approximate the potential profile by a series of potential steps at $x_1, \ldots, x_i, \ldots x_N$, and determine the transfer matrices $M^{(i)}; i = 1, \ldots, N$. The product of all these matrices is the the transfer matrix M that connects the amplitudes A, B left of the potential profile, to those on the right F, G. This matrix then aloows one to calculate the transmission and reflection coefficients.

In principle, one has all the freedom in choosing the grid points $x_1, \ldots, x_i, \ldots x_N$ and the positions $V(\xi_i)$; $x_i \leq \xi_i \leq x_{i+1}; i = 1, \ldots, N-1$ at which the plateaus of the potential approximation are placed.

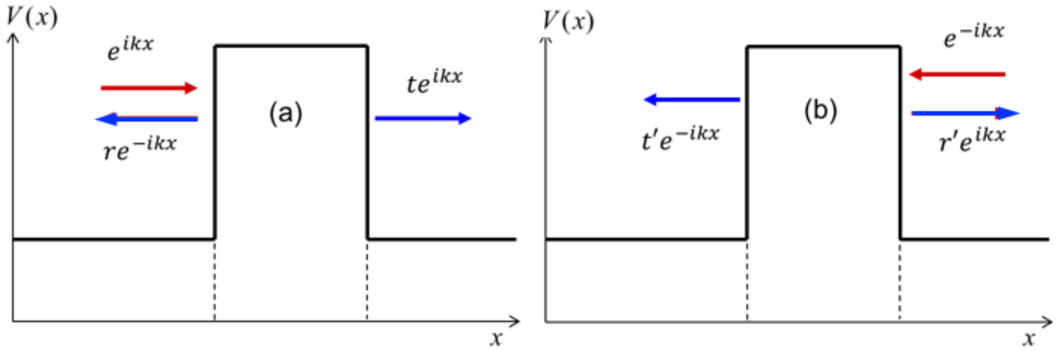
The good news is that all of these choices converge to a unique transfer matrix in the limit of an infinite dense grid, which gives a unique solution to the Schrodinger equation [provided your potential is a healthy one; mathematicians can most likely come up with potentials for which the algorithm fails, but those are unhealthy potentials; best to put them in quarantine].

The bad news is that the quality of the approximation of a grid with a finite density, depends on the positioning of the points $x_1, \ldots, x_i, \ldots x_N$ and the points ξ_i; $x_i \leq \xi_i \leq x_{i+1}; i = 1, \ldots, N-1$, read section 1.2 of the lecture notes.



There is worse news. The transfer matrix algorithm is very versatile, and it works in many cases very well. Sometimes, however, it fails, in particular when it comes to describing tunneling through thick and/or high barriers, read section 1.3 of the lecture notes. We will explore some of this in the project. Meanwhile, there is a remedie against this particular numerical instability; it is called the scattering matrix approach.

Scattering matrix (S-matrix)



relating amplitudes of outgoing waves to incoming waves

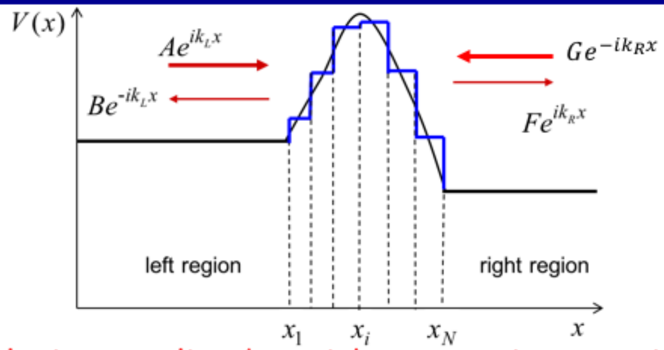
$$S = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix}$$

$T = |t|^2 = |S_{21}|^2$ transmission coefficient

$R = |r|^2 = |S_{11}|^2$ reflection coefficient

The scattering matrix is similar in spirit to the transfer matrix. Whereas the latter connects amplitudes of waves right of the barrier to those left of the barrier, the scattering matric connects amplitudes of outgoing waves (blue arrows in the above picures) to amplitudes of incoming waves (read arrows in the pictures above). There are two possible incoming waves, $\exp[ikx]$ from the left, and $\exp[-ikx]$ from the right, and each can be reflected and transmitted with coefficients r,t and r',t', respectively. These coefficients can be expressed in terms of the matrix elements of the transmission matrix if you like, read section 2 of the lecture notes.

Scattering matrix algorithm, barrier of any shape



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hep sun foordeil"

relating amplitudes with scattering matrix

$$\binom{B}{F} = S^{(1)} \circ S^{(2)} \circ \cdots \circ S^{(N-1)} \circ S^{(N)} \binom{A}{G} \equiv S \binom{A}{G}$$

disadvantage: $S^{(1)} \circ S^{(2)}$ much more complicated than just matrix product

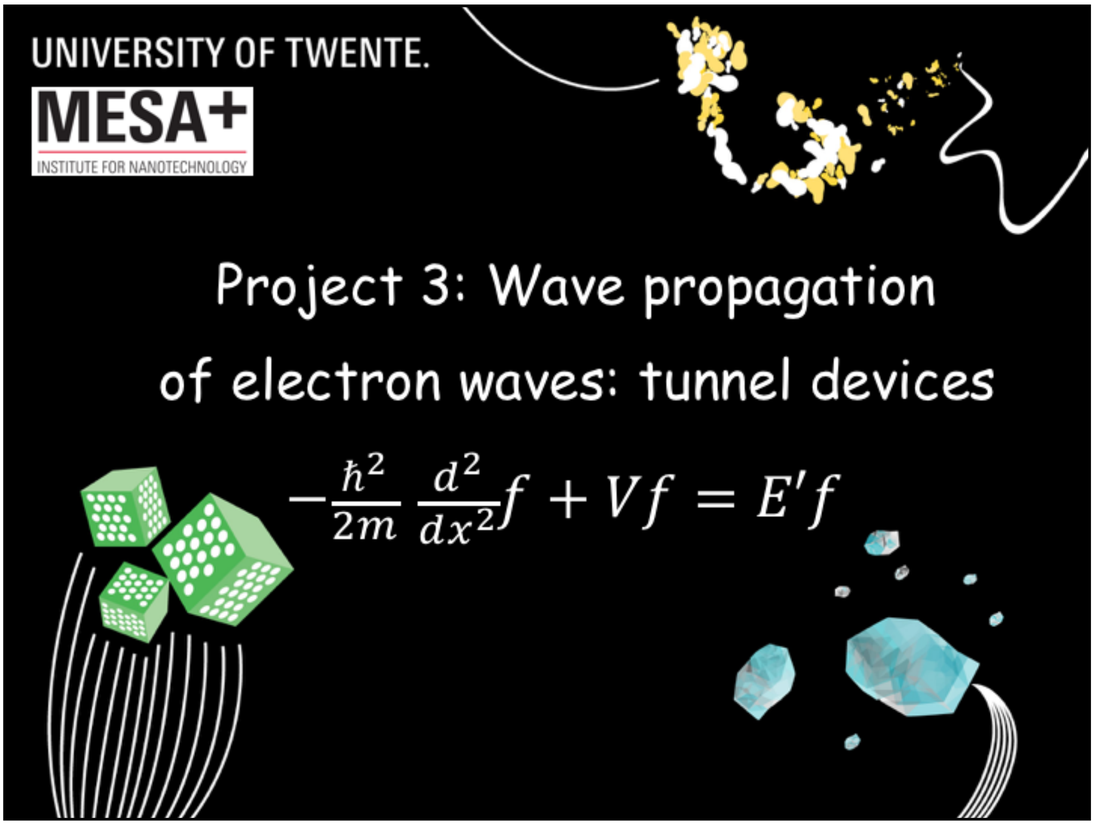
advantage: S-matrix algorithm more stable than transfer matrix algorithm

One can use the same "grid and step" approach as for the transmission matrix algorithm, to approximate a potential profile by a series of potential steps. The amplitudes B of the refflected wave, and F of the transmitted waves, can then be obtained from the amplitudes A, G of the incoming waves, by combining the scattering matrices of the individual steps.

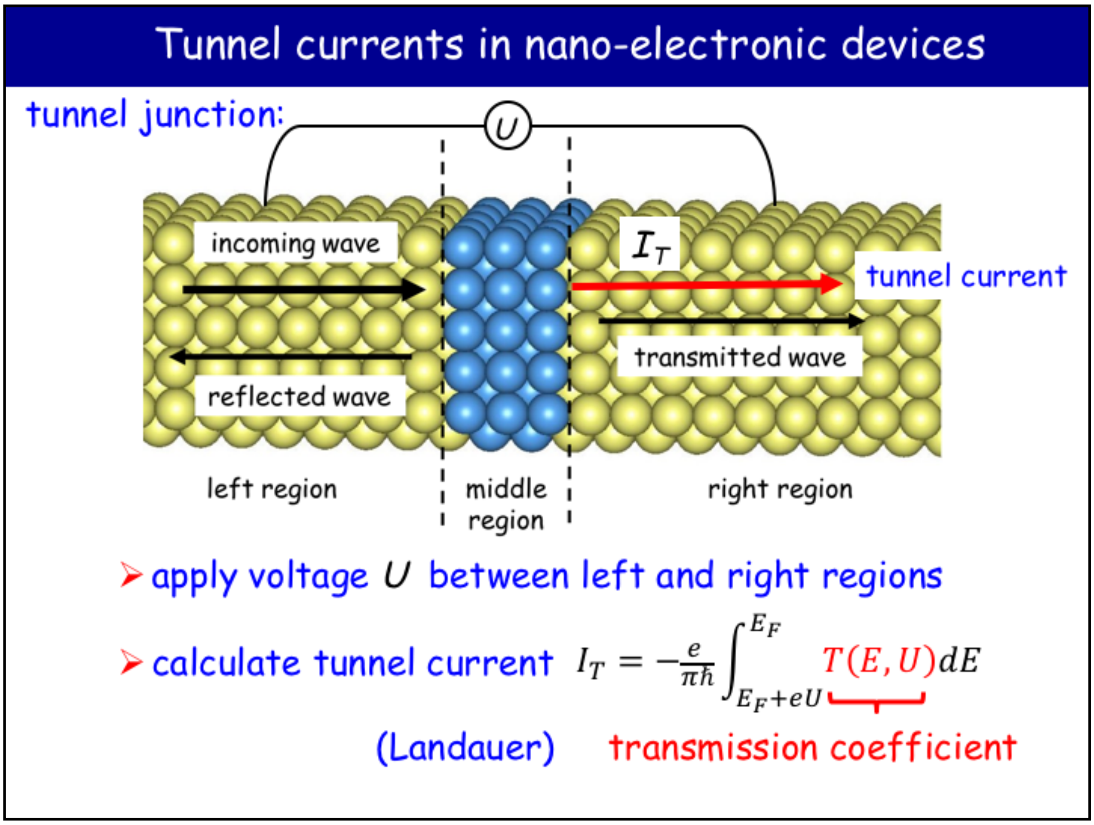
The disadvantage of this method is that the "product" of two scattering matrices $S^{(1)} \circ S^{(2)}$ is more complicated than just a matrix product (for the product rule, see section 2.1 of the lecture notes).

The advantage however is that the algorithm is stable, see section 2.2 of the lecture notes.

[A second advantage is that the elements of the scattering matrix have a direct physical interpretation, see section 3 of the lecture notes.]



In our projects we will explore how potential barriers of different kinds transport (i.e., reflect and transmit) electron waves. To make sure that you don’t think that this is all abstarct physics, we will calculate the electron transport properties, i.e., the current-voltage characteristics, of some (more or less) realistic tunnel devices.



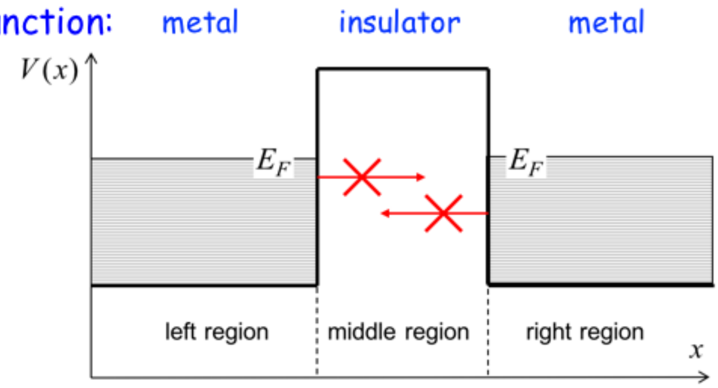
Consider a device called a tunnel junction. It consists of a insulating layer (usually a few nm's thick; indicated as "middle region" above), sandwiched between two metals (indicated as "left region" and "right region" above). The drawing above is not entirely representative; we wish to consider the case where the regions are "infinite" (at least μm's) in the directions perpendicular to the tunnel current.

Apply a voltage U between the left and the right regions. This will give rise to a tunnel current I_T. The Landauer formula states that this tunnel current can be expressed in therms of the transmission coefficients T of the individual electron waves. One has to assume that all scattering is elastic, which means that no energy is "lost" in scattering, i.e., the scattered electrons emerge at the same energy as the incoming electrons. This implies a low temperature, as electron-phonon scattering is a major source for inelastic scattering, and at low temperature the number of phonons is low. The expression given here is actually for zero temperature. An extension to finite temperature is possible, but we won't bother about that in this project.

For a background in quantum currents, quantum conduction, and a derivation of the Landauer formula, see sections 5 and 6 of the lecture notes.

One-dimensional tunnel junction

tunnel junction:

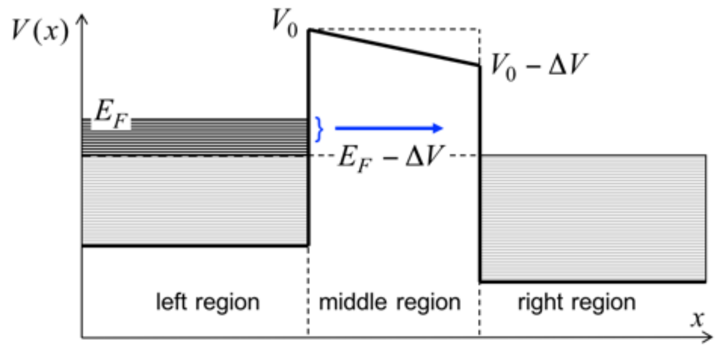


- zero bias: no current between left and right regions

The idea behind the Landauer formula in a nut shell. At zero bias the whole system is in equilibrium, which means that the Fermi level (or electrochemical potential, if you wish to be pedantic) left and right of the barrier are the same. No electron can cross the barrier, because it keeps the same energy (elastic scattering only), and on the other side of the barrier it find this energy level already occupied by other electrons. The Pauli principle then forbids such a multiple occupancy.

Landauer formula

tunnel junction: metal insulator metal



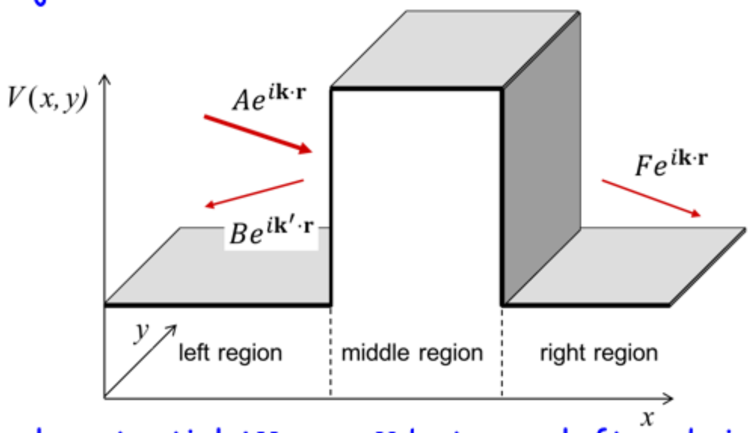
- apply potential $\Delta V = -eU$ between left and right regions
- calculate tunnel current $$I_T = -\frac{e}{\pi\hbar}\int_{E_F-\Delta V}^{E_F} \underbrace{T(E,\Delta V)}_{\text{transmission coefficient}} dE$$

(Landauer)

If we apply a bias $\Delta V = -eU$ between left and right regions, the whole right region is lowered in energy by ΔV with respect to the left region. Note that, because the middle region is an insulator, the whole potential drop takes place over this region. In particular, the Fermi level of the right region is now at $E_F - \Delta V$. This means that in the left region, electrons with energies between $E_F - \Delta V$ and E_F now find an empty level in the right region. The block by the Pauli principle is lifted for these electrons. They can tunnel from the left to the right region and contribute to the tunnel current. The probability that they reach the other side is determined by the transmission coefficient T, which obviously depends upon the energy of the electrons. It also depends on ΔV, as the shape of the barrier depends on it. [For the prefactor $e/\pi\hbar$ you should have a look at the detailed derivation of the Landauer formula in section 6 of the lecture notes.]

Three-dimensional tunnel junction

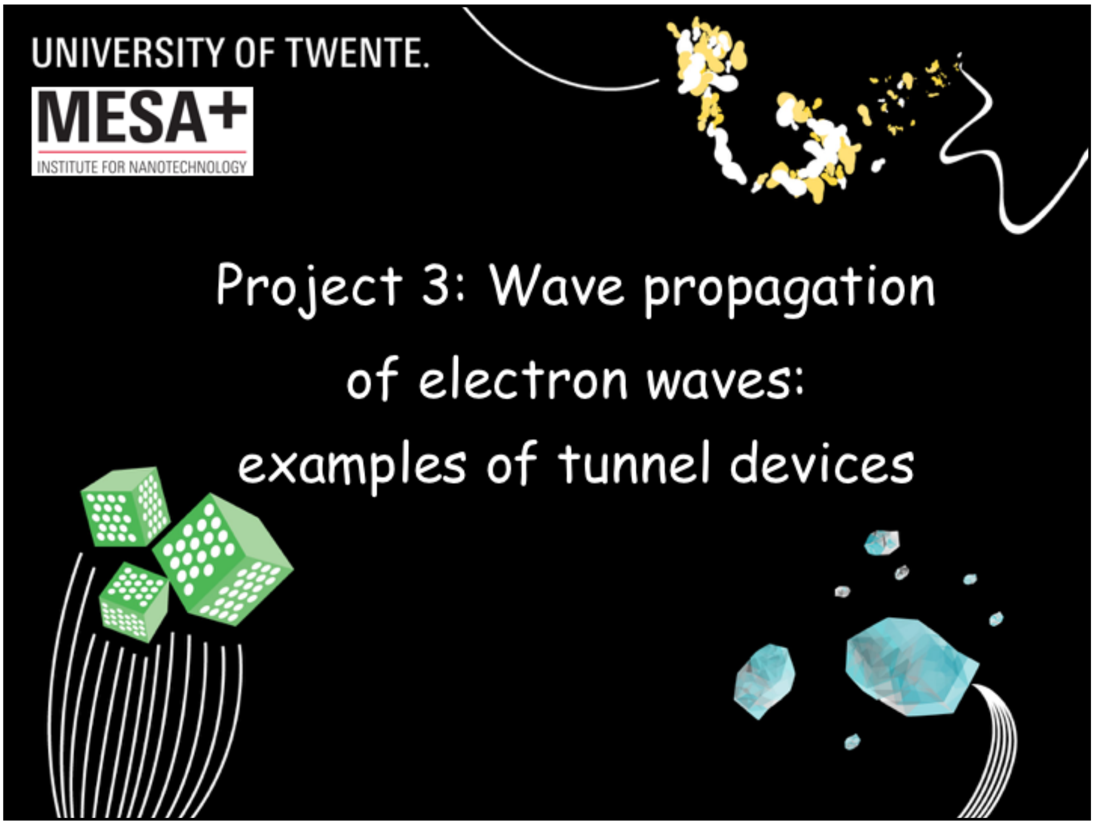
tunnel junction: metal insulator metal



- apply potential $\Delta V = -eU$ between left and right regions
- calculate tunnel current (Tsu-Esaki)

$$I_T = -\frac{em}{\pi^2\hbar^3}\left[\Delta V \int_0^{E_F-\Delta V} T(E_x, \Delta V)\,dE_x + \int_{E_F-\Delta V}^{E_F} (E_F - E_x)T(E_x, \Delta V)\,dE_x\right]$$

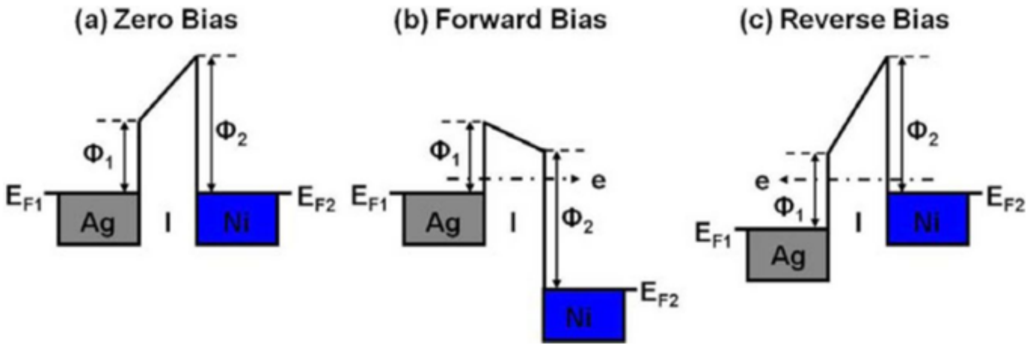
It is possible to generalize the one-dimensional Landauer formula to three dimensions, see section 7 of the lecture notes. For a system consisting of (homogeneous) layers, the result is called the Tsu-Esaki equation.



What the title says: some examples of tunnel devices we will consider in this project.

Metal-Insulator-Metal (MIM) diodes

tunnel junction: metal-insulator-metal: Ag-NiO-Ni

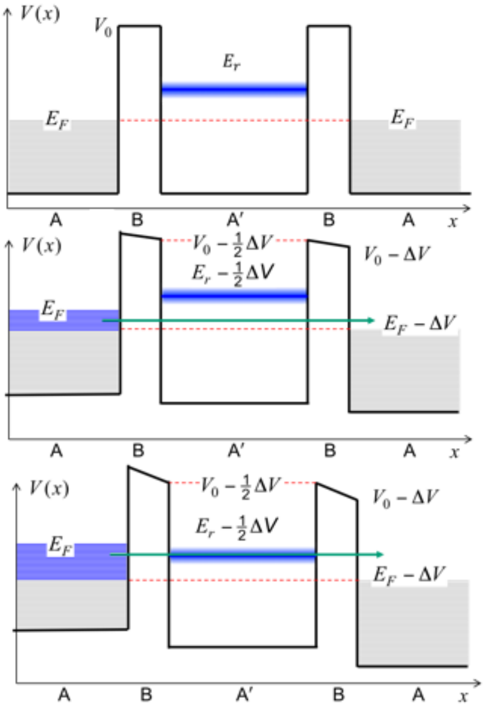


no current "large" current "small" current

- non-linear I/V characteristics
- applications: fast switching (THz), flat panel thin-film diodes

One device we will consider is called a metal-insulator-metal (MIM) diode, see section 8 of the lecture notes. It consists of two metals with a different work function Φ_1 and Φ_2 (essential that they are different), separated by a thin insulator layer (usually an oxide). A MIM device has highly non-linear I/V characteristics. It would be nice if these characteristics are asymmetric, i.e., if one would have a sizeable difference between the current with forward bias and that with reverse bias. That way one has a diode. It turns out that MIMs can switch very fast, and are very cheap to make over a large area.

Resonant-Tunneling Diodes (RTDs) (Esaki)



double barrier potential

- quasi-bound state

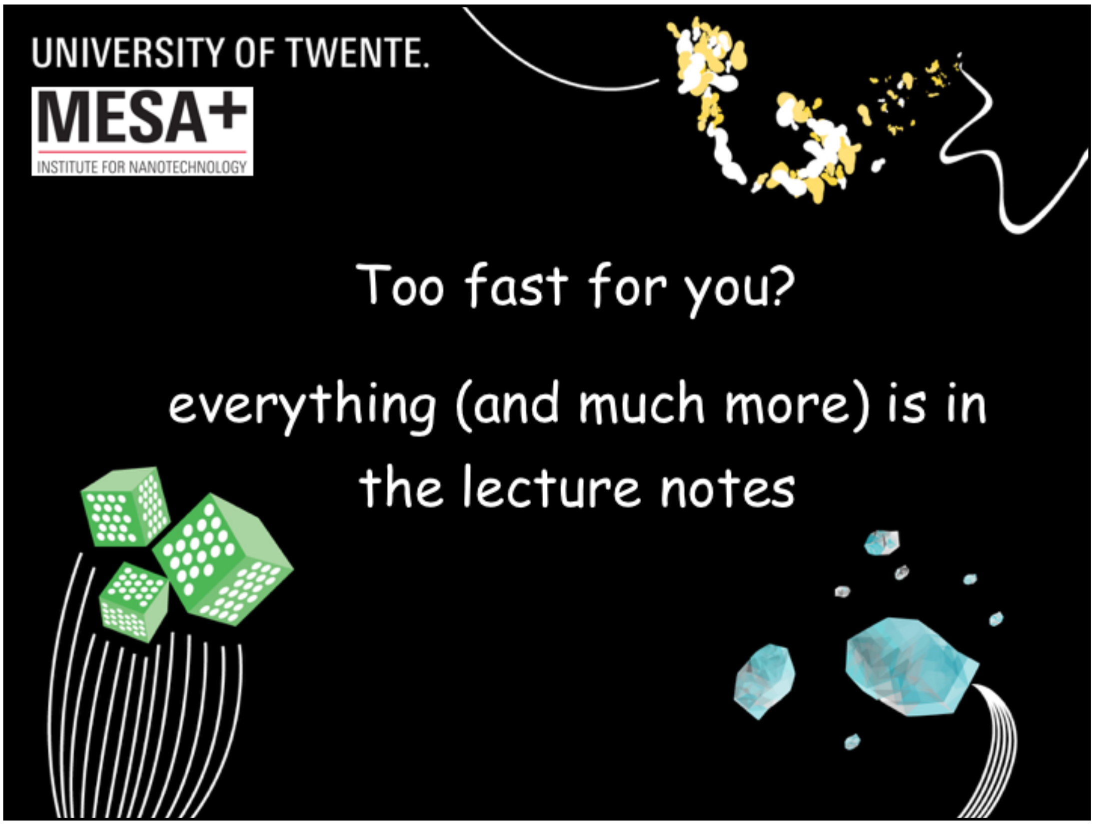
apply potential $\Delta V = -eU$

- non-resonant condition: small tunnel current

apply potential $\Delta V = -eU$

- resonant condition: large tunnel current

Another device is called a resonant tunneling diode (RTD), see section 9 of the lecture notes. It is basically a double barrier structure, made by stacking layers of different semiconductors by epitaxial growth. The region between the two barriers supports so-called quasi-bound states (section 9). Under resonant conditions, these states transport electrons from the left to the right side of the device, which gives rise to a relatively large tunneling current. Under non-resonant conditions, these states are too high (or too low) in energy, i.e. outside the energy window $E_F - \Delta V$ to E_F, to participate in the transmission, making the current relatively low.



I hope everything is in the lecture notes.