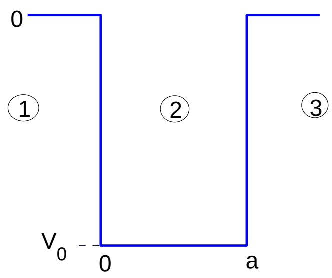
Beräkningsverktyg, lösning till övn. 3.4c i 'Kvantvärldens fenomen'

In regions 1 and 3:

$$\frac{-\hbar^2}{2m}\phi'' + 0\phi = E\phi \quad \Longrightarrow$$

$$\phi'' = -\frac{2mE}{\hbar^2}\phi = -k^2\phi \quad (k^2 = \frac{2mE}{\hbar^2})$$



Solutions of the form (with no returned wave in region 3):

$$\begin{aligned} \phi_1 &= Ae^{ikx} + Be^{-ikx} \quad \Longrightarrow \quad \phi_1' = Aike^{ikx} + B(-ik)e^{-ikx} \\ \phi_3 &= Fe^{ikx} \quad \Longrightarrow \quad \phi_1' = F(ik)e^{ikx} \end{aligned}$$

In region 2:

$$\frac{-\hbar^2}{2m}\phi'' - V_0\phi = E\phi \quad \Longrightarrow \quad \phi'' = -\frac{2m(E+V_0)}{\hbar^2}\phi = -K^2\phi \quad (k^2 = \frac{2m(E+V_0)}{\hbar^2})$$

with the same type of solution as in regions 1 and 3:

$$\phi_2 = Ce^{iKx} + De^{-iKx} \quad \Longrightarrow \quad \phi_2' = C(iK)e^{iKx} + D(-iK)e^{-iKx}$$

Continuity of the wave-function and its first derivative at $x = 0$ and $x = a$:

$$\begin{aligned} A + B &= C + D \\ kA - kB &= kC - kD \\ Ce^{iKa} + De^{-iKa} &= Fe^{ika} \\ C(iK)e^{iKa} + D(-iK)e^{-iKa} &= F(ik)e^{ika} \end{aligned}$$

With the amplitudes in units of A

$$\begin{cases} +(B/A) & -(C/A) & -(D/A) & & = -1 \\ -k(B/A) & -K(C/A) & +K(D/A) & & = -k \\ & +e^{iKa}(C/A) & +e^{-iKa}(D/A) & -e^{ika}(F/A) & = 0 \\ & +iKe^{iKa}(C/A) & -iKe^{-iKa}(C/A) & -ike^{ika}(E/A) & = 0 \end{cases}$$

corresponding to the system

$$\mathbf{Ax} = \mathbf{y}$$

with

$$\mathbf{A} = \begin{bmatrix} 1 & -1 & -1 & 0 \\ -k & -K & K & 0 \\ 0 & e^{iKa} & e^{-iKa} & -e^{ika} \\ 0 & +Ke^{iKa}) & -Ke^{-iKa} & -ke^{ika} \end{bmatrix}, \quad \mathbf{x} = \begin{bmatrix} B/A \\ C/A \\ D/A \\ F/A \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} -1 \\ k \\ 0 \\ 0 \end{bmatrix}$$

The probability current of the incoming wave in region 1 is given as $(\hbar k/m)|A|^2$ and for the outcoming wave in region 3 $(\hbar k/m)|F|^2$. This gives the transmission coefficient:

$$T = T(E) = \frac{(\hbar k/m)|F|^2}{(\hbar k/m)|A|^2} = \left|\frac{F}{A}\right|^2$$

Constants:

$$k = \sqrt{\frac{2mE}{\hbar^2}} = \sqrt{\frac{2mc^2E}{(\hbar c)^2}}$$

With $\hbar c = 197.3271$ eV nm and $m_ec^2 = 510.99910^3$ eV and with E in eV, k will be in units of [1/nm]. The only difference for K compared with k is that E is replaced by $(E + V_0)$, where $V_0 = 5$ eV.

It is possible to find an analytic solution (see p. 201, G. Ohlén, Kvantvärldens fenomen:

$$T = \left(1 + \frac{V_0}{4E\left(E+V_0\right)}\sin^2\left(ka\right)\right)^{-1}$$

Matlab-fil för lösning av uppgiften:

```
% transmission.m  inlamningsuppgift 2, deluppgift 1, ht 2005

clear all
close all

L=50; % antal punkter i energivektorn.
E_vector = linspace(eps,10,L);
T_vector=zeros(L,1);

a = 1; % [nm]
mC2=510999; % [eV]
hbarC=197.3271; % [eV nm]
V0=5; % [eV]

for j = 1:L
    E=E_vector(j);
    K = sqrt( (2*mC2*(E+V0))/(hbarC^2) );
    k = sqrt( (2*mC2*(E))/(hbarC^2) );

    y = [-1 -k 0 0]'; % ekvationssystemets högerled

    A = [            % matris for koefficienterna till de fyra obekanta "B, C, D, E".
        1 -1 -1 0;
        -k -K K 0;
        0 exp(i*K*a) exp(-i*K*a) -exp(i*k*a);
        0 K*exp(i*K*a) -K*exp(-i*K*a) -k*exp(i*k*a)
    ];
   % x = A\y; % losningen till ekvation systemet.
   % x = inv(A)*y;
   x = A\y

    T_vector(j) = abs(x(4))^2;
   % 4.e positionen i x vektorn är amplituden för den transmitterade vagen.
end

plot (E_vector, T_vector,'-')
hold on

% Jämförelse med analytisk beräkning
Ein_vector = linspace(eps,10,200);
k_vector=sqrt( 2*mC2*(Ein_vector+V0)/hbarC^2 );
analytic=1./(1 + V0^2./(4*Ein_vector.*(Ein_vector+V0)).* sin(k_vector*a).^2 );
% sidan 201 i 'Kvantvärldens fenomen'.
plot(Ein_vector,analytic,'r--')
axis([0 10 0 1.4])
legend('Numeriskt beraknad','Analytisk formel, sid. 201','Location','NW')
xlabel('Energi [e.V.]','fontsize',15)
ylabel('Transmitans','fontsize',15)
```