Documentation on the java^{TM} packet

Scattering at a potential well

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Abstract

This documentation describes the usage of this Mathematica Player Notebook and provides the theory that is groundwork of it. It illustrates the scattering of a particle ray at a potential well.

The notebook has been modified and optimized for the usage in lectures within the „OWL-project e-Module zur Veranschaulichung der Theoretischen Physik“. The original version is taken from the *Wolfram Demonstration Project*[1][2]

[1] http://demonstrations.wolfram.com/ScatteringByASquareWellPotential/
[2] Translated to english by Stanislav Ax 15.03.2014

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Imprint

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Project: „Offensive Wissen durch Lernen“
„e-Module zur Veranschaulichung der Theoretischen Physik“
Head of the project: *Prof. Dr. Eckehard Schöll, PhD*
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1 Description

Many experiments in physics (especially in the high energy physics) are based on the interaction between a particle ray („beam“) and another particle („target“). Informations about the interacting forces(energy, etc.) can be obtained by investigating the scattered beam. Scattering is distinguished from general particle interactions by the demand that the impact on the target is elastic and the initial and the final state are consisting of the same particles(explicit: no „generation“of new particles during the impact). In this Mathematica Player Notebook the particle beam is scattered at the one-dimensional potential well.

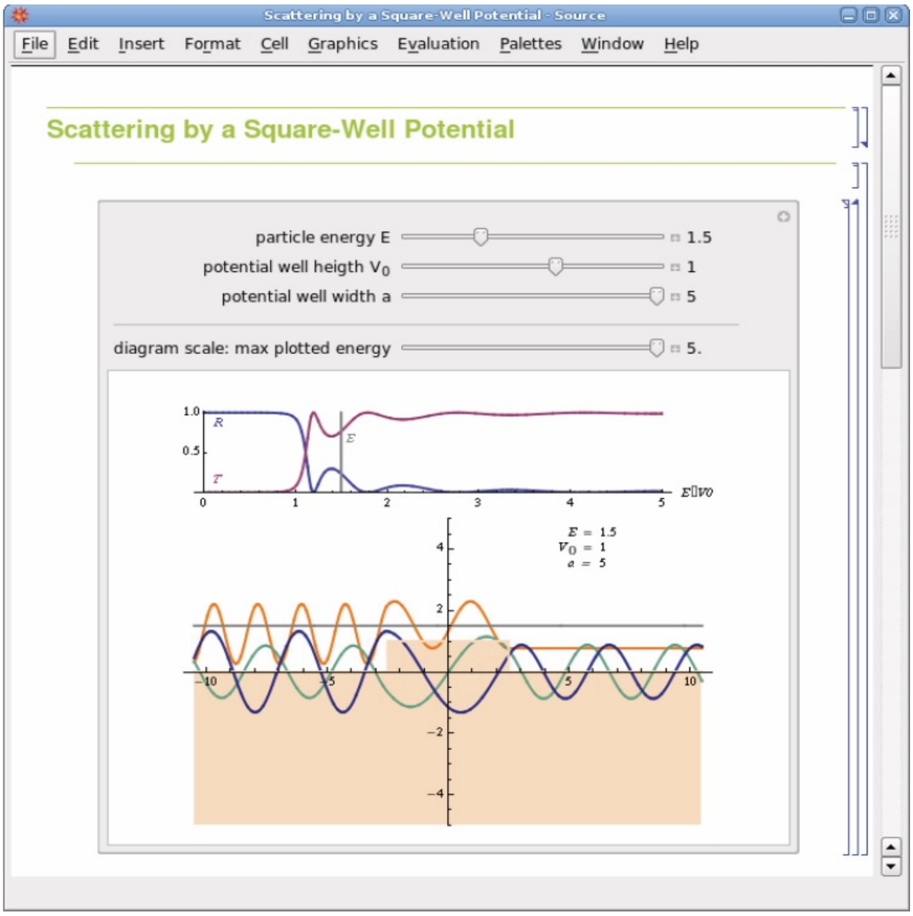

Figure 1: screenshot of the Notebook opened in Mathematica 6.0

One part of the beam will be transmitted and the other one will be reflected since the beam has properties of a wave. The reflected part is drawn in light orange. To keep things simple only a stationary state with energy E like in the calculation for the one-dimensional potential well will be used. Usually a particle is considered as wave packet, it is a superposition of the single waves with differing frequencies. The reflected beam interfers with the incoming wave on the left side of the potential well. This cause inteference patterns to appear.

Two charts are contained within the window with the animations. With the adjustments chosen in the figure the upper chart is showing the reflection(violet) and the transmission(blue) in dependence of the energy. The chart shows well how big the influence of the reflected respectively the transmitted wave is. A grey transom indicates the set energy. In the lower window a local representation of the wave and the potential well is shown. The real part of the wave is plotted in blue, the imaginary part in green and the absolute square in orange.

Two special cases may occur. The complete reflection and the complete transmission. The complete transmission occures if the condition $aq = n\pi$ is fulfilled (“a„wall thickness, q wave vector in the potential well)(see section theory). This is the same condition like for the eigen conditions in the infinetly high potential well.

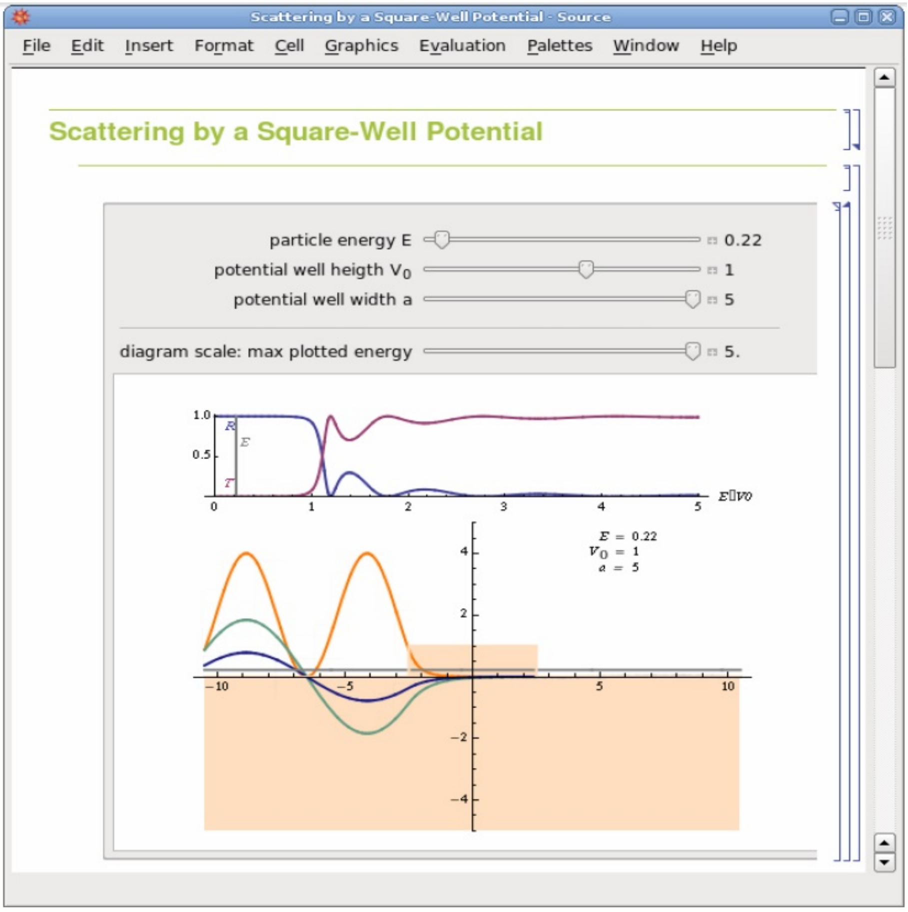

Figure 2: screenshot during complete reflection

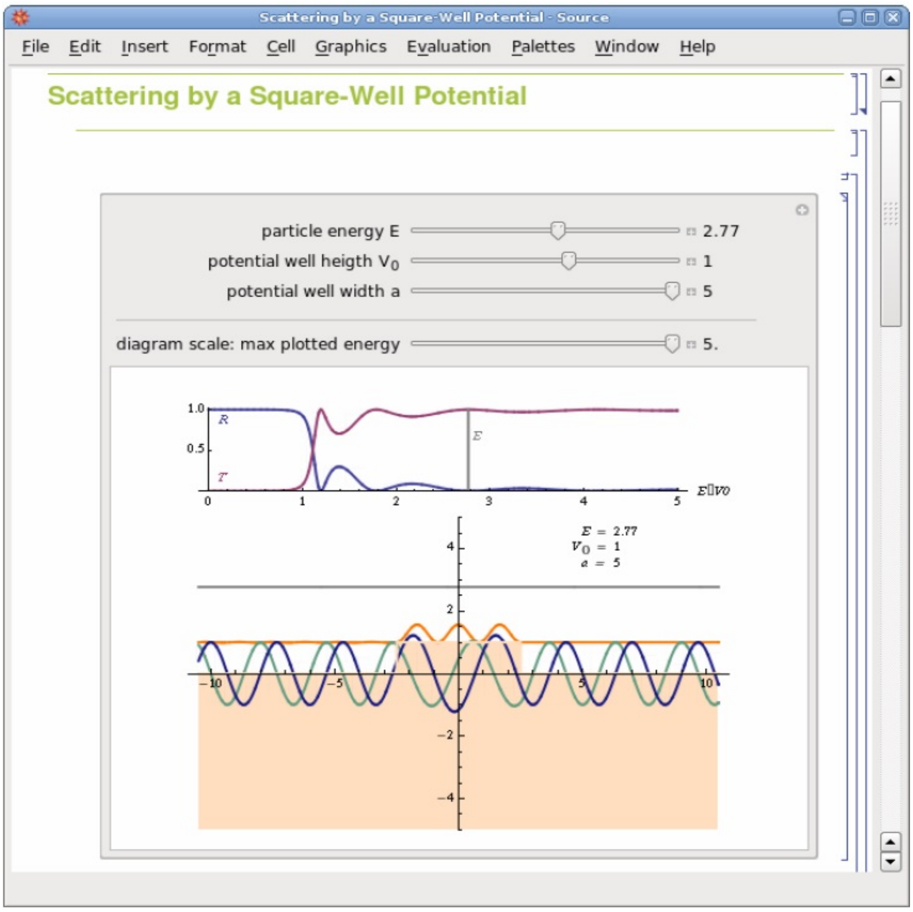

Figure 3: screenshot during complete transmission

2 Usage

Four controls may be manipulated by the user. The controls are for manipulating the particle energy E, the height of the potential well, the width of the well and the energy scaling. In contrary to the original notebook one can choose positive values for the height of the potential well, this way one obtains a potential barrier. By manipulating the controls one can observe the change of the reflection and transmission properties.

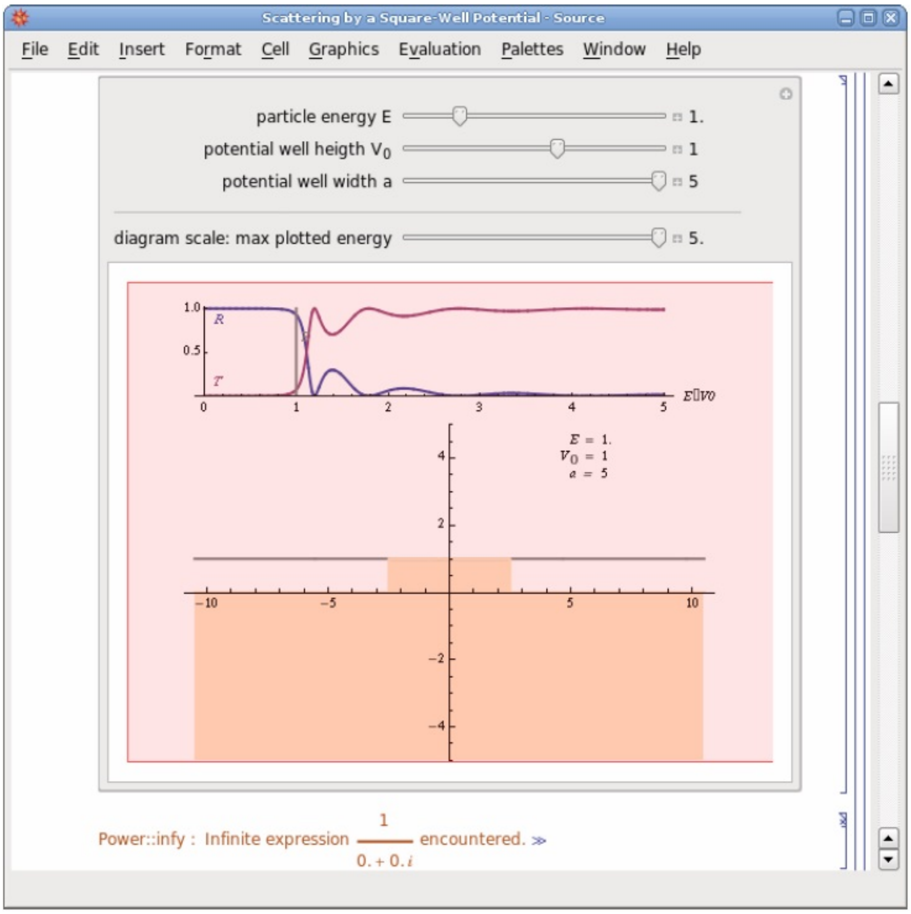

Figure 4: screenshot of the Notebook during $E = V_0$ division through zero

3 Program

Changing the controls in the program cause the equations for the three regions (reflection region/ region with potential unequal zero/ transmission region) to be recalculated. Since the initial condition (energy of the wave) is known, a simple formula can be used to calculate the wave function (see next chapter: theory)

4 Theory

According to the Schrödinger equation the time development of a wave is given by

$$\Psi(x,t) = \phi(x) e^{-\frac{Et}{\hbar}} \tag{1}$$

In which $\phi(x)$ is the solution of the Schrödinger equation

$$[-\frac{\hbar^2}{2m}\Delta + V(x)]\phi(x) = E\phi(x) \tag{2}$$

The incoming wave ia a plane wave with amplitude equal to one

$$\phi(x) = e^{ikx} \tag{3}$$

The incoming wave solves equation 2 with $E = \frac{\hbar^2 k^2}{2m}$ in which E corresponds to the energy of the wave.

Equation 2 is rewritable into the following equation if the potential V is constant

$$\frac{d^2}{dx^2}\phi(x) + \frac{2m}{\hbar^2}(E - V)\phi(x) = 0 \tag{4}$$

The general solution of this differential equation for E>V is given by

$$\phi(x) = Ae^{ikx} + Be^{-ikx} \tag{5}$$

When A and B are complex numbers. For E<V follows

$$\phi(x) = A'e^{qx} + B'e^{-qx} \tag{6}$$

$(A', B' \in \mathbb{C})$ Only the continuation condition of $\phi(x)$ is needed to determine the coefficients A and B within the three regions.

$$\phi_I(x) = e^{ikx} + Be^{-ikx} \tag{7}$$

$$\phi_{II}(x) = A'e^{iqx} + B'e^{-iqx} \tag{8}$$

$$\phi_{III}(x) = A''e^{ikx} \tag{9}$$

$B'' = 0$ since no incoming wave is existing within the third region.

Together with the continuation condition it follows

$$\phi_I(k, q) = e^{ikx} + e^{-ikx}\frac{e^{-ika}(k^2 - q^2)sin(aq)}{2ikqcos(aq) + (k^2 + q^2)sin(aq)} \tag{10}$$

with $E - V = \frac{\hbar^2 q^2}{2m}$

$$\phi_{II}(k,q) = \frac{2ikqe^{-ik}}{2ikqcos(aq) + (k^2+q^2)sin(aq)} \frac{q+k}{2q} e^{\frac{i(k-q)}{2}} e^{iqx} + \tag{11}$$

$$\frac{2ikqe^{-ik}}{2ikqcos(aq) + (k^2+q^2)sin(aq)} \frac{q-k}{2q} e^{\frac{i(k+q)}{2}} e^{-iqx} \tag{12}$$

and

$$\phi_{III}(k,q) = e^{ikx} \frac{2ikqe^{-ika}}{2ikqcos(aq) + (k^2+q^2)sin(aq)} \tag{13}$$

This derivation is also shown in QM[1] (Complement H_I: Stationary states of a particle in one-dimensional square potentials). For further reading QM[2] (Chapter VIII: An elementary approach to the quantum theory of scattering by a potential) is recommendable.
textbfLiterature

[1] Franck Laloë Claude Cohen-Tannoudji, Bernard Diu. Quantum Mechanics, Volume One (Translation of Mecanique quantique I). Wiley-VCH, New York, London, Sidney, Toronto, 1977.

[2] Franck Laloë Claude Cohen-Tannoudji, Bernard Diu. Quantum Mechanics, Volume Two (Translation of Mecanique quantique II). Wiley-VCH, New York, London, Sidney, Toronto, 1977.

Literatur

[1] Franck Laloë Claude Cohen-Tannoudji, Bernard Diu. *Quantum Mechanics, Volume One (Translation of Mecanique quantique I)*. Wiley-VCH, New York, London, Sidney, Toronto, 1977.

[2] Franck Laloë Claude Cohen-Tannoudji, Bernard Diu. *Quantum Mechanics, Volume Two (Translation of Mecanique quantique II)*. Wiley-VCH, New York, London, Sidney, Toronto, 1977.

A Quelltexte

Anmerkung: Im Notebook ist $\hbar$ und m gleich eins gesetzt.

Listing 1: modifiziertes Notebook

```
V[x_, V0_, a_] := V0 (UnitStep[x + a/2] - UnitStep[x - a/2])
(*The "amplitude" of the reflected wave *)

RR[k_, q_] := (\[ExponentialE]^(-\[ImaginaryI] k) (k^2 - q^2) Sin[
   q])/(2 \[ImaginaryI] k q Cos[q] + (k^2 + q^2) Sin[q])
(*The "amplitude" of the transmitted wave.*)

TT[k_, q_] :=  \[ImaginaryI] 2 k q (\[ExponentialE]^(-\[ImaginaryI] \
k)) /(2 \[ImaginaryI] k q Cos[q] + (k^2 + q^2) Sin[q])
(* The amplitudes of the waves inside the well *)

AA[k_, q_] := TT[k, q] (q + k)/(2 q) Exp[I (k - q)/2]
BB[k_, q_] := TT[k, q] (q - k)/(2 q) Exp[I (k + q)/2]
\[Psi][x_, En_, V0_, a_] := Module[
  {z = x/a, k = a Sqrt[2 En], q = a Sqrt[2 (En - V0)], Rv, Tv, Av,
   Bv},
  Rv = RR[k, q];
  Tv = TT[k, q];
  Av = AA[k, q];
  Bv = BB[k, q];
  Which[
   z < -1/2, Exp[I k z] + Rv*Exp[-I k z],
   Abs[z] \[LessEqual] 1/2, Av*Exp[I q x/a] + Bv*Exp[-I q z],
   z > 1/2, Tv*Exp[I k z]]
  ]
TransmitanceAndReflectance[En_, V0_, a_] := Module[
  {k = a Sqrt[2 En], q = a Sqrt[2 (En - V0)], Rv, Tv, Av, Bv},
  Rv = Abs[RR[k, q]];
  Tv = Abs[TT[k, q]];
  {Rv^2, Tv^2}                                          ]
xmax         = 10.5;
ymax         = 5.0;
energyMax = 5.0;

Manipulate[
 Column[{Plot[
    TransmitanceAndReflectance[z*Abs[V0] (*Energy*), V0, a] //
     Evaluate,
    {z, 0, ymax/Abs[V0]},
    PlotRange \[Rule] {0, 1.02},
    BaseStyle \[Rule] Directive[Thick],
    PlotStyle \[Rule]
     {ColorData[1, 1],
      ColorData[1, 2],
      Gray
       },
    Ticks \[Rule] {Automatic, {{0.5, "0.5"}, {1.0, "1.0"}}},
    AxesLabel \[Rule] {Style["E/V0", Italic],  ""},
    AspectRatio \[Rule] 1/5.5,
    ImageSize \[Rule] {490, 100},
```

```
    Exclusions \[Rule] None,
    Epilog \[Rule] {ColorData[1, 1],
      Text[Style["R", Italic], {0.1/Abs[V0], 0.95}, {−1, +1}],
      ColorData[1, 2],
      Text[Style["T", Italic], {0.1/Abs[V0], 0.05}, {−1, −1}],
      Gray, Line[{{En/Abs[V0], 1}, {En/Abs[V0], 0}}],
      Text[Style["E", Italic], {(En + 0.1)/Abs[V0], 0.65}]}
         ],
   Plot[
    With[{val = \[Psi][x, En, V0, a]},
      {Abs[val]^2, Re[val], Im[val], En, V[x, V0, a]}
          ] // Evaluate,
    {x, −xmax, xmax},
    PlotRange \[Rule] {−ymax, ymax},
    PlotPoints \[Rule] 75,
    PlotStyle \[Rule]
     {RGBColor[1, .47, 0],
      RGBColor[.38, .61, .51],
      RGBColor[.1, .1, .51],
      Gray,
      Lighter[Orange, .75]
        },
    Filling \[Rule] {5 \[Rule] Bottom},
    FillingStyle \[Rule] Lighter[Orange, .75],
    BaseStyle \[Rule] Directive[Thick],
    ImageSize \[Rule] {490, 250},
    Exclusions \[Rule] None,
    Epilog \[Rule] {Text[
       Row[{Style["E", Italic], " = "}], {0.6 xmax,
        0.9 ymax}, {+1, 0}],
      Text[ToString[En], {0.6 xmax, 0.9 ymax}, {−1, 0}],
      Text[
       Row[{Subscript[Style["V", Italic], 0], " = "}], {0.6 xmax,
        0.8 ymax}, {+1, 0}],
      Text[ToString[V0], {0.6 xmax, 0.8 ymax}, {−1, 0}],
      Text[
       Style[Row[{Style["a", Italic], " = "}], Italic], {0.6 xmax,
        0.7 ymax}, {+1, 0}],
      Text[ToString[a], {0.6 xmax, 0.7 ymax}, {−1, 0}]
                        }
              ]
   }, Center],
 {{En, 1.5, "particle energy E"}, 0, 5,
  Appearance \[Rule] "Labeled"},
 {{V0, 1, Row[{"potential well heigth ", Subscript["V", 0]}]}, −5, 5,
  Appearance \[Rule] "Labeled"},
 {{a, 5, "potential well width a"}, 0.5, 5,
  Appearance \[Rule] "Labeled"},
 Delimiter,
 {{ymax, 5, "diagram scale: max plotted energy"}, 0.5, 5,
  Appearance \[Rule] "Labeled"},
 SaveDefinitions \[Rule] True
                              ]
```

Listing 2: original Notebook

```
V[x_, V0_, a_] := V0 (UnitStep[x + a/2] − UnitStep[x − a/2])
(*The "amplitude" of the reflected wave *)

RR[k_, q_] := (\[ExponentialE]^(−\[ImaginaryI] k) (k^2 − q^2) Sin[
   q])/(2 \[ImaginaryI] k q Cos[q] + (k^2 + q^2) Sin[q])
(*The "amplitude" of the transmitted wave.*)

TT[k_, q_] :=  \[ImaginaryI] 2 k q (\[ExponentialE]^(−\[ImaginaryI] \
k)) /(2 \[ImaginaryI] k q Cos[q] + (k^2 + q^2) Sin[q])
(* The amplitudes of the waves inside the well *)

AA[k_, q_] := TT[k, q] (q + k)/(2 q) Exp[I (k − q)/2]
BB[k_, q_] := TT[k, q] (q − k)/(2 q) Exp[I (k + q)/2]
\[Psi][x_, En_, V0_, a_] := Module[
  {z = x/a, k = a Sqrt[2 En], q = a Sqrt[2 (En − V0)], Rv, Tv, Av,
```

```
    Bv},
   Rv = RR[k, q];
   Tv = TT[k, q];
   Av = AA[k, q];
   Bv = BB[k, q];
   Which[
    z < -1/2, Exp[I k z] + Rv*Exp[-I k z],
    Abs[z] \[LessEqual] 1/2, Av*Exp[I q x/a] + Bv*Exp[-I q z],
    z > 1/2, Tv*Exp[I k z]]
   ]
TransmitanceAndReflectance[En_, V0_, a_] := Module[
   {k = a Sqrt[2 En], q = a Sqrt[2 (En - V0)], Rv, Tv, Av, Bv},
   Rv = Abs[RR[k, q]];
   Tv = Abs[TT[k, q]];
   {Rv^2, Tv^2}                                    ]
xmax          = 10.5;
ymax          = 5.0;
energyMax = 5.0;



Manipulate[
 Column[{Plot[
     TransmitanceAndReflectance[z (*Energy*), V0, a] // Evaluate,
     {z, 0, energyMax},
     PlotRange \[Rule] {0, 1.02},
     BaseStyle \[Rule] Directive[Thick],
     Ticks \[Rule] {Automatic, {{0.5, "0.5"}, {1.0, "1.0"}}},
     AxesLabel \[Rule] {Style["E", Italic], ""},
     AspectRatio \[Rule] 1/5.5,
     ImageSize \[Rule] {490, 100},
     Exclusions \[Rule] None,
     Epilog \[Rule] {ColorData[1, 1],
       Text[Style["R", Italic], {0.1, 0.95}, {-1, +1}],
       ColorData[1, 2],
       Text[Style["T", Italic], {0.1, 0.05}, {-1, -1}]}
          ],
    Plot[
     With[{val = \[Psi][x, En, V0, a]},
       {Abs[val]^2, Re[val], Im[val], En, V[x, V0, a]}
         ] // Evaluate,
     {x, -xmax, xmax},
     PlotRange \[Rule] {-ymax, ymax},
     PlotPoints \[Rule] 75,
     PlotStyle \[Rule]
      {RGBColor[1, .47, 0],
       RGBColor[.38, .61, .51],
       RGBColor[.1, .1, .51],
       Gray,
       Lighter[Orange, .75]
        },
     Filling \[Rule] {5 \[Rule] Bottom},
     FillingStyle \[Rule] Lighter[Orange, .75],
     BaseStyle \[Rule] Directive[Thick],
     ImageSize \[Rule] {490, 250},
     Exclusions \[Rule] None,
     Epilog \[Rule] {Text[
        Row[{Style["E", Italic], " = "}], {0.6 xmax,
         0.9 ymax}, {+1, 0}],
       Text[ToString[En], {0.6 xmax, 0.9 ymax}, {-1, 0}],
       Text[
        Row[{Subscript[Style["V", Italic], 0], " = "}], {0.6 xmax,
         0.8 ymax}, {+1, 0}],
       Text[ToString[V0], {0.6 xmax, 0.8 ymax}, {-1, 0}],
       Text[
        Style[Row[{Style["a", Italic], " = "}], Italic], {0.6 xmax,
         0.7 ymax}, {+1, 0}],
       Text[ToString[a], {0.6 xmax, 0.7 ymax}, {-1, 0}]
                      }
             ]
    }, Center],
 {{En, 1.5, "particle energy E"}, 0, 5,
```

```
 Appearance \[Rule] "Labeled"},
{{V0, -1, Row[{"potential well depth ", Subscript["V", 0]}]}, -5, -1,
  Appearance \[Rule] "Labeled"},
{{a, 5, "potential well width a"}, 0.5, 5,
 Appearance \[Rule] "Labeled"},
SaveDefinitions \[Rule] True
                         ]
```