Schroedinger equation

1.Ecuatia Schroedinger unidimensionala

Introducere

```
ClearAll["Global`*"]
Off[General::spell, General::spell1]
```

Particula intr-o groapa finita de potential

- **Cerem pachetele de programe de care avem nevoie**

```
Needs["Graphics`"];
```

- **Rezolvarea problemei:**

```
Clear["Global`*"];
```

- **pasul 1 Stabilim forma solutiei generale a ecuatie lui Schrodinger**

```
eq1 = 0 == (V - En) ψ[x] - ħ^2 ψ''[x] / (2 m);
```

$$\text{eq1} = 0 == (V - \text{En})\,\psi[x] - \frac{\hbar^2\,\psi''[x]}{2\,m};$$

```
eq2 = eq1 /. V → 0
```

$$0 == -\text{En}\,\psi[x] - \frac{\hbar^2\,\psi''[x]}{2\,m}$$

```
krule = En → ℏ^2 k^2/(2 m);
```

```
schrod = Solve[eq2 /. krule, ψ''[x] ][[1, 1]] /. Rule → Equal
```

$$\psi''[x] == -k^2\,\psi[x]$$

```
dsol= DSolve[schrod,ψ,x][[1,1]]
```

```
ψ → Function[{x}, C[1] Cos[k x] + C[2] Sin[k x]]
```

■ pasul 2→Solutia para

```
sol1 = Reduce[{ψ[0] == 0, ψ[a] == 0} /. dsol]
```

```
(Sin[a k] == 0 && C[1] == 0) || (Sin[a k] ≠ 0 && C[2] == 0 && C[1] == 0)
```

$$En == \frac{k^2\,\hbar^2}{2\,m}\ /.\ k \to \frac{(n-1/2)\,\pi}{a}$$

$$En == \frac{\left(-\frac{1}{2}+n\right)^2 \pi^2\,\hbar^2}{2\,a^2\,m}$$

$$En\ ==\ \frac{\left(-\frac{1}{2}+n\right)^2 \pi^2\,\hbar^2}{2\,a^2\,m}$$

$$En == \frac{\left(-\frac{1}{2}+n\right)^2 \mathrm{Null}\,\pi^2\,\hbar^2}{2\,a^2\,m}$$

$$\psi p[x\_,\ n\_] = \psi[x]\ /.\ dsol\ /.\ \left\{C[1] \to 0,\ k \to \frac{(n-1/2)\,\pi}{a}\right\}$$

$$C[2]\ \mathrm{Sin}\left[\frac{\left(-\frac{1}{2}+n\right)\pi\,x}{a}\right]$$

```
normEq =
 1 == Integrate[ψp[x, n]^2, {x, -a, a}] //
   Simplify[#, Element[n, Integers]] & // Solve[#, C[2]][[2, 1]] &
```

$$C[2] \to \frac{1}{\sqrt{a}}$$

```
ψpara[x_, n_] = ψp[x, n] /. normEq // Simplify
```

$$\frac{\mathrm{Sin}\left[\frac{\left(-\frac{1}{2}+n\right)\pi x}{a}\right]}{\sqrt{a}}$$

```
ψpara[x, n]
```

$$\frac{\mathrm{Sin}\left[\frac{\left(-\frac{1}{2}+n\right)\pi x}{a}\right]}{\sqrt{a}}$$

```
En[n_] = ((n - 1 / 2) π / a)^2 * ħ^2 / (2 m)
```

$$\frac{\left(-\frac{1}{2}+n\right)^2 \pi^2 \hbar^2}{2 a^2 m}$$

■ pasul 3→Reprezentarea grafica a solutiilor impare

```
table= Table[Integrate[ψpara[x,i]ψpara[x,j],{x,-a,a}],{i,4},{j,4}];
```

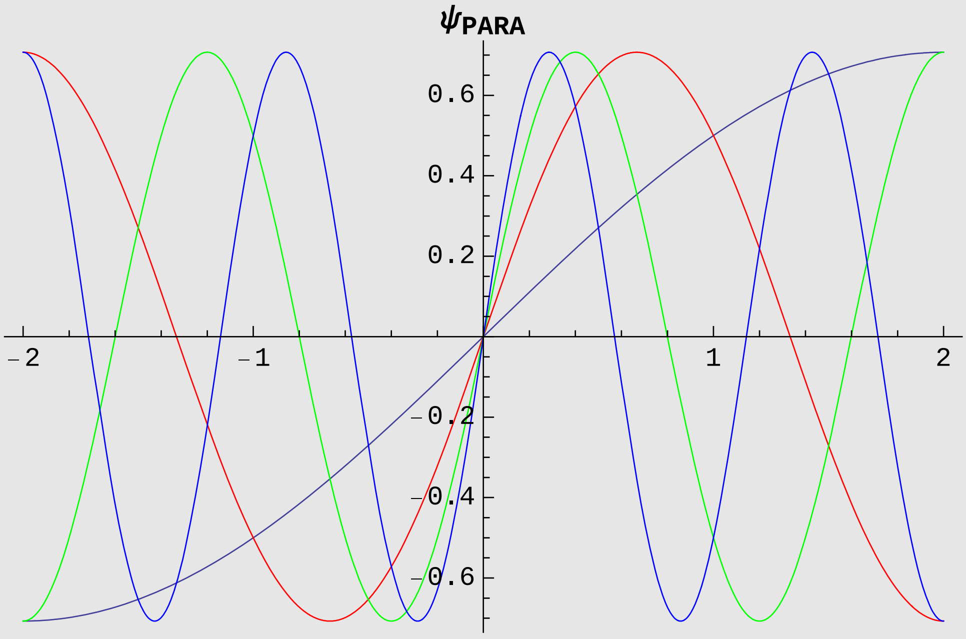
```
TableForm[table,
 TableHeadings → {Table[ψpara[i], {i, 4}], Table[ψpara[j], {j, 4}]}]
```

	ψpara[1]	ψpara[2]	ψpara[3]	ψpara[4]
ψpara[1]	1	0	0	0
ψpara[2]	0	1	0	0
ψpara[3]	0	0	1	0
ψpara[4]	0	0	0	1

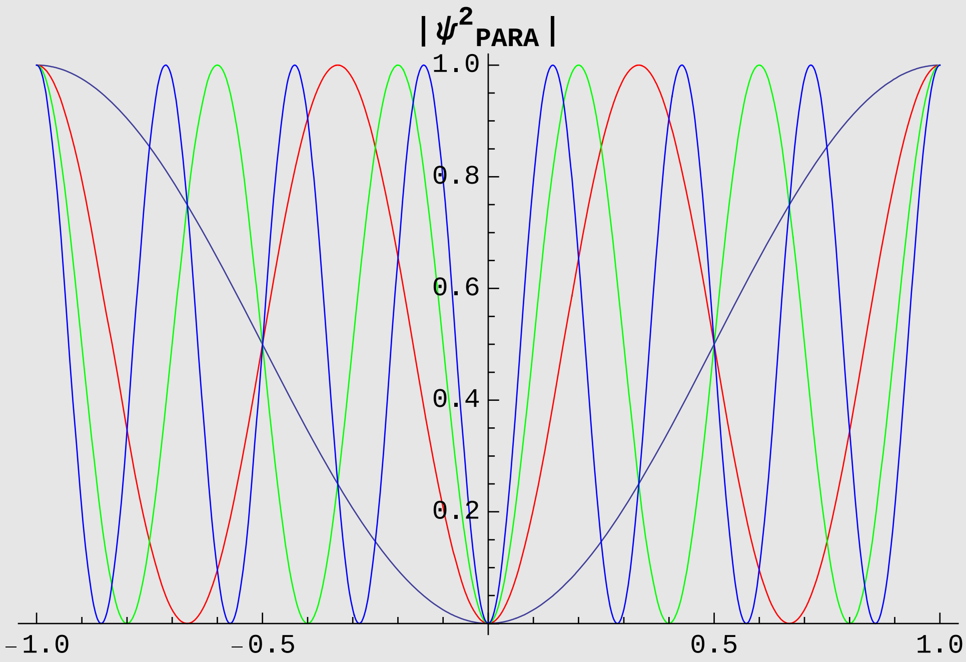
```
table = Table[En[i], {i, 4}]
```

$$\left\{\frac{\pi^2\hbar^2}{8\,a^2\,m},\ \frac{9\,\pi^2\hbar^2}{8\,a^2\,m},\ \frac{25\,\pi^2\hbar^2}{8\,a^2\,m},\ \frac{49\,\pi^2\hbar^2}{8\,a^2\,m}\right\}$$

```
Plot[Evaluate[Table[ψpara[x, n], {n, 4}] /. {a → 2}], {x, -2, 2},
 PlotStyle → {{}, RGBColor[1, 0, 0], RGBColor[0, 1, 0],
   RGBColor[0, 0, 1]},
 PlotLabel → Style[ψPARA, FontSize → 14, FontWeight → Bold]]
```



```
Plot[Evaluate[Table[ψpara[x, n]^2, {n, 4}] /. {a → 1}], {x, -1, 1},
 PlotStyle → {{}, RGBColor[1, 0, 0], RGBColor[0, 1, 0],
   RGBColor[0, 0, 1]},
 PlotLabel →
  Style[
   "|\!\(\*SubscriptBox[SuperscriptBox[\(ψ\), \(2\)], \(PARA\)]\)|",
   FontSize → 14, FontWeight → Bold]]
```



■ **pasul 4→Solutia impara**

```
sol1 = Reduce[{ψ[0] == 0, ψ[a] == 0} /. dsol]
```

```
(Sin[a k] == 0 && C[1] == 0) || (Sin[a k] ≠ 0 && C[2] == 0 && C[1] == 0)
```

$$\text{Enp} == \frac{k^2 \hbar^2}{2 m} \text{ /. } k \to \frac{n \pi}{a}$$

$$\text{Enp} == \frac{n^2 \pi^2 \hbar^2}{2 a^2 m}$$

```
ψimpara[x_, n_] = ψ[x ] /. dsol /. {C[2] → 0, k → n π/a}
```

$C[1]\,\mathrm{Cos}\left[\frac{n\,\pi\,x}{a}\right]$

```
normEq =
 1 == Integrate[ψimpara[x, n]^2, {x, -a, a}] //
   Simplify[#, Element[n, Integers]] & // Solve[#, C[1]][[2, 1 ]] &
```

$C[1]\to\frac{1}{\sqrt{a}}$

```
ψimpara[x_, n_] = ψimpara[x, n] /. normEq // Simplify
```

$\frac{\mathrm{Cos}\left[\frac{n\,\pi\,x}{a}\right]}{\sqrt{a}}$

```
Enim[n_] = (n π/a)^2 * ħ^2/(2 m)
```

$\frac{n^2\,\pi^2\,\hbar^2}{2\,a^2\,m}$

- **pasul 3→Reprezentarea grafica a solutiilor impare**

```
table= Table[Integrate[ψimpara[x,i]ψimpara[x,j],{x,-a,a}],{i,4},{j,4}];
```

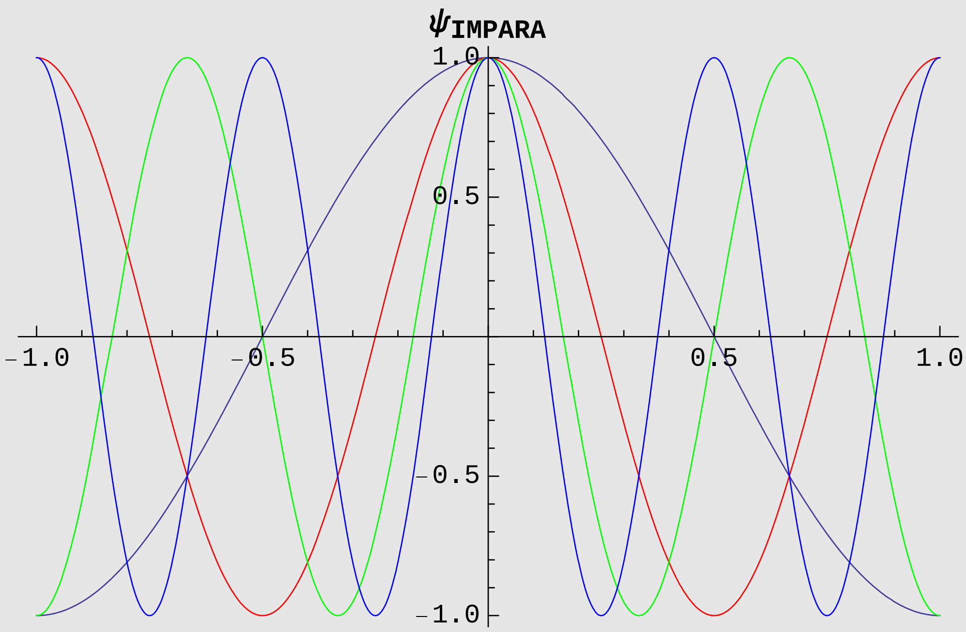
```
TableForm[table,
 TableHeadings → {Table[ψimpara[i], {i, 4}], Table[ψimpara[j], {j, 4}]}]
```

	ψimpara[1]	ψimpara[2]	ψimpara[3]	ψimpara[4]
ψimpara[1]	1	0	0	0
ψimpara[2]	0	1	0	0
ψimpara[3]	0	0	1	0
ψimpara[4]	0	0	0	1

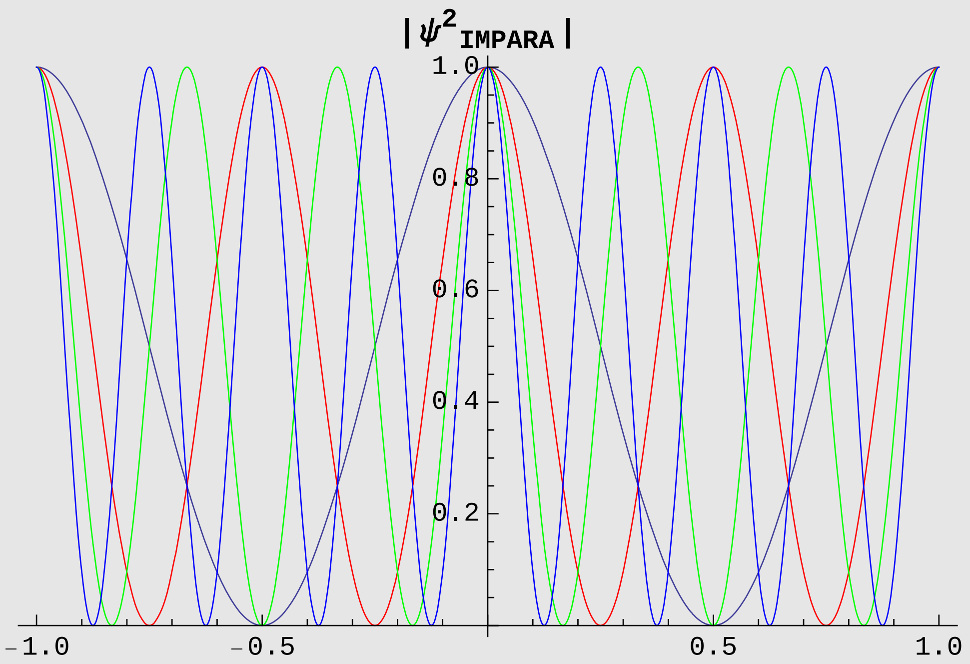
```
tableim = Table[Enim[i], {i, 4}]
```

$$\left\{\frac{\pi^2 \hbar^2}{2 a^2 m}, \frac{2 \pi^2 \hbar^2}{a^2 m}, \frac{9 \pi^2 \hbar^2}{2 a^2 m}, \frac{8 \pi^2 \hbar^2}{a^2 m}\right\}$$

```
Plot[Evaluate[Table[ψimpara[x, n], {n, 4}] /. {a → 1}], {x, -1, 1},
 PlotStyle → {{}, RGBColor[1, 0, 0], RGBColor[0, 1, 0],
   RGBColor[0, 0, 1]},
 PlotLabel → Style["\!\(\*SubscriptBox[\(ψ\), \(IMPARA\)]\)",
   FontSize → 14, FontWeight → Bold]]
```



```
Plot[Evaluate[Table[ψimpara[x, n]^2, {n, 4}] /. {a → 1}], {x, -1, 1},
 PlotStyle → {{}, RGBColor[1, 0, 0], RGBColor[0, 1, 0],
   RGBColor[0, 0, 1]},
 PlotLabel →
  Style[
   "|\!\(\*SubscriptBox[SuperscriptBox[\(ψ\), \(2\)],
     \(IMPARA\)]\)|", FontSize → 14, FontWeight → Bold]]
```



Particula intr-o groapa finita de potential

■ Solution

```
Clear["Global`*"];
```

■ Pas 1

$$\text{schrodeq} = 0 == (V - \text{En})\,\psi[x] - \frac{\hbar^2\,\psi''[x]}{2\,m};$$

$$\text{EWrule} = \left\{\text{En} \to \frac{\text{kW}^2\,\hbar^2}{2\,m} + V\right\};$$

```
ψ[x] /. DSolve[schrodeq, ψ[x], x][[1, 1]] /. EWrule // ExpToTrig //
  Simplify // PowerExpand
```

$(C[1] + C[2]) \mathrm{Cos}[kW\, x] + i\, (C[1] - C[2]) \mathrm{Sin}[kW\, x]$

$$\mathbf{kWrule} = kW \to \frac{\sqrt{2}\sqrt{m\,(En - V)}}{\hbar}\ /.\ V \to -V0\ /.\ En \to -Wn$$

$$kW \to \frac{\sqrt{2}\sqrt{m\,(V0 - Wn)}}{\hbar}$$

```
ψW[x_] = cSym Cos[kW x] + cAsym Sin[kW x];
```

$$\mathbf{ELRrule} = \left\{En \to \frac{kLR^2\,\hbar^2}{2\,m}\right\};$$

```
ψ[x] /. DSolve[schrodeq, ψ[x], x][[1, 1]] /. V → 0 /. ELRrule //
  Simplify // PowerExpand
```

$e^{i\,kLR\,x}\,C[1] + e^{-i\,kLR\,x}\,C[2]$

$$\mathbf{kLRrule} = kLR \to \frac{\sqrt{2}\sqrt{En\,m}}{\hbar}\ /.\ En \to -Wn\ //\ PowerExpand$$

$$kLR \to \frac{i\sqrt{2}\sqrt{m}\sqrt{Wn}}{\hbar}$$

$$\mathbf{qLRrule} = qLR \to \frac{\sqrt{2}\sqrt{m\,Wn}}{\hbar};$$

```
ψ[x] /. DSolve[schrodeq, ψ[x], x][[1, 1]] /. V → 0 /. ELRrule /.
   kLR → I qLR // Simplify // PowerExpand
```

$e^{qLR\,x}\,C[1] + e^{-qLR\,x}\,C[2]$

$\psi R[x\_] = cR\, E^{-qLR\,x}$;   (*x>a*)

$\psi L[x\_] = cL\, E^{+qLR\,x}$;   (*x<-a*)

pas 2

```
eq1= {  (ψL[ x]-ψW[ x]==0)  /. {x-> -a},
        (ψW[ x]-ψR[ x]==0)  /. {x-> +a},
        (ψL'[x]-ψW'[x]==0)  /. {x-> -a},
        (ψW'[x]-ψR'[x]==0)  /. {x-> +a}  }
```

$\{cL\, e^{-a\, qLR} - cSym\, Cos[a\, kW] + cAsym\, Sin[a\, kW] == 0,$
$-cR\, e^{-a\, qLR} + cSym\, Cos[a\, kW] + cAsym\, Sin[a\, kW] == 0,$
$cL\, e^{-a\, qLR}\, qLR - cAsym\, kW\, Cos[a\, kW] - cSym\, kW\, Sin[a\, kW] == 0,$
$cR\, e^{-a\, qLR}\, qLR + cAsym\, kW\, Cos[a\, kW] - cSym\, kW\, Sin[a\, kW] == 0\}$

```
Column[eq2 = eq1 /. cAsym → 0]
```

$cL\, e^{-a\, qLR} - cSym\, Cos[a\, kW] == 0$
$-cR\, e^{-a\, qLR} + cSym\, Cos[a\, kW] == 0$
$cL\, e^{-a\, qLR}\, qLR - cSym\, kW\, Sin[a\, kW] == 0$
$cR\, e^{-a\, qLR}\, qLR - cSym\, kW\, Sin[a\, kW] == 0$

```
eq3 =
 Reduce[Flatten[{eq2, cL ≠ 0, cR ≠ 0, kW ≠ 0, qLR ≠ 0, cSym ≠ 0,
    Cos[a kW] ≠ 0}], {cL, cR}]
```

$Cos[a\, kW] \neq 0\, \&\&\, cSym\, e^{a\, qLR}\, kW\, Sin[a\, kW] \neq 0\, \&\&\, qLR == kW\, Tan[a\, kW]\, \&\&$
$cL == cSym\, e^{a\, qLR}\, Cos[a\, kW]\, \&\&\, cR == cSym\, e^{a\, qLR}\, Cos[a\, kW]$

```
MatrixForm[{eq3}]
```

$(Cos[a\, kW] \neq 0\, \&\&\, cSym\, e^{a\, qLR}\, kW\, Sin[a\, kW] \neq 0\, \&\&\, qLR == kW\, Tan[a\, kW]\, \&\&\, cL == cSym\, e^{a}$

```
symSol = Solve[eq3 , {cL, cR} ] // Simplify // Flatten
```

$\{cL \to cSym\, e^{a\, qLR}\, Cos[a\, kW],\, cR \to cSym\, e^{a\, qLR}\, Cos[a\, kW]\}$

```
symEn = Tan[a kW] ==  qLR / kW;
```

```
eq4 =
 Reduce[Flatten[{eq1 /. cSym → 0, cL ≠ 0, cR ≠ 0, kW ≠ 0, qLR ≠ 0,
    cAsym ≠ 0, Cos[a kW] ≠ 0}], {cL, cR}]
Column[eq4]
```

$cAsym\, e^{a\, kW \operatorname{Cot}[a\, kW]}\, kW \operatorname{Cos}[a\, kW] \operatorname{Sin}[a\, kW] \neq 0\ \&\&\ qLR == -kW \operatorname{Cot}[a\, kW]\ \&\&$
$cL == -cAsym\, e^{-a\, kW \operatorname{Cot}[a\, kW]} \operatorname{Sin}[a\, kW]\ \&\&\ cR == cAsym\, e^{a\, qLR} \operatorname{Sin}[a\, kW]$

$\operatorname{Column}\Big[cAsym\, e^{a\, kW \operatorname{Cot}[a\, kW]}\, kW \operatorname{Cos}[a\, kW] \operatorname{Sin}[a\, kW] \neq 0\ \&\&\ qLR == -kW \operatorname{Cot}[a\, kW]\ \&\&$
$cL == -cAsym\, e^{-a\, kW \operatorname{Cot}[a\, kW]} \operatorname{Sin}[a\, kW]\ \&\&\ cR == cAsym\, e^{a\, qLR} \operatorname{Sin}[a\, kW]\Big]$

```
asymSol = Solve[eq4 , {cL, cR} ] // Simplify // Flatten
```

$\{cR \to cAsym\, e^{a\, qLR} \operatorname{Sin}[a\, kW],\ cL \to -cAsym\, e^{-a\, kW \operatorname{Cot}[a\, kW]} \operatorname{Sin}[a\, kW]\}$

```
asymEn = Tan[a kW] == - kW / qLR;
```

pas 3

```
values = {a → 1, m → 1, ℏ → 1, V0 → { 100, 200, 500, ∞}} ;
```

$$nRule = Wn \to V0 - \frac{n^2 \pi^2 \hbar^2}{8 a^2 m};$$

$$kRules = \left\{kW \to \frac{\sqrt{2\, m\, (V0 - Wn)}}{\hbar},\ qLR \to \frac{\sqrt{2\, (Wn)\, m}}{\hbar}\right\};$$

```
eq5 =symEn/.kRules /.nRule//PowerExpand
```

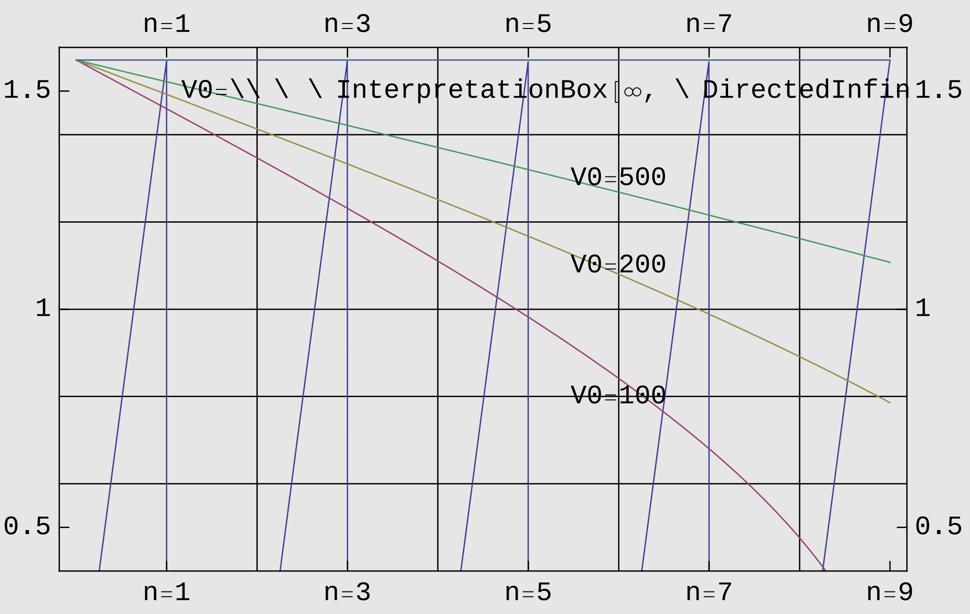
$$\operatorname{Tan}\left[\frac{n\, \pi}{2}\right] == \frac{2 \sqrt{2}\, a \sqrt{m} \sqrt{V0 - \frac{n^2 \pi^2 \hbar^2}{8\, a^2\, m}}}{n\, \pi\, \hbar}$$

```
pt1 = Plot[{ArcTan[eq5[[1]]], ArcTan[eq5[[2]]]} /. values // Evaluate,
   {n, 0, 9 },
   Frame → True,
   FrameTicks →
    {{{1, "n=1"}, {3, "n=3"}, {5, "n=5"}, {7, "n=7"}, {9, "n=9"}},
     {0, 0.5, 1, 1.5}},
   PlotRange → {.4, 1.6},
   DisplayFunction → Identity];
```

Plot::exclul : $\left\{\mathrm{Re}\left[\frac{\infty}{\mathrm{Sign}[n]}\right]-0\right\}$ must be a list of equalities or real–valued functions. ≫

```
text = {
   Text[ "V0=\\ \ \ InterpretationBox[∞, \ DirectedInfinity[\ 1]]",
    {6, 1.5}],
   Text[ "V0=500", {6, 1.3}],
   Text[ "V0=200", {6, 1.1}],
   Text[ "V0=100", {6, 0.8}]};
```

```
Show[pt1, Graphics[text], GridLines → Automatic,
 DisplayFunction → $DisplayFunction]
```

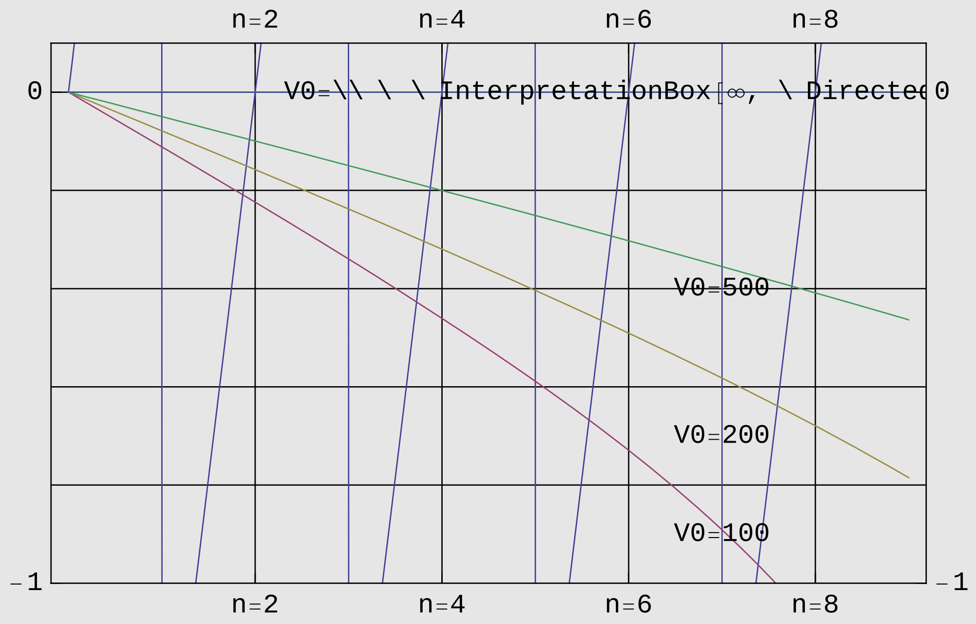



```
eq6 =asymEn/.kRules /.nRule//PowerExpand
```

$$\mathrm{Tan}\left[\frac{n\,\pi}{2}\right] == -\frac{n\,\pi\,\hbar}{2\sqrt{2}\,a\sqrt{m}\,\sqrt{V0-\frac{n^2\,\pi^2\,\hbar^2}{8\,a^2\,m}}}$$

```
text = {
    Text[ "V0=\\ \ \ InterpretationBox[∞, \ DirectedInfinity[\ 1]]",
     {7, 0}],
    Text[ "V0=500", {7, -.4}],
    Text[ "V0=200", {7, -.7}], Text[ "V0=100", {7, -.9 }]};
```

```
Plot[Evaluate[{ArcTan[eq6[[1]]], ArcTan[eq6[[2]]]} /. values],
 {n, 0.`, 9}, Frame → True,
 FrameTicks → {{{2, "n=2"}, {4, "n=4"}, {6, "n=6"}, {8, "n=8"}},
   {-1.5`, -1, 0, 0.5`, 1, 1.5`}}, PlotRange → {-1, 0.1`},
 GridLines → Automatic, Epilog → text]
```



■ **pas 4**

```
nValues[eq_, potential_, guess_] :=
 (n /. FindRoot[eq /. {m → 1, a → 1, ħ → 1, V0 → potential} // Evaluate,
      {n, guess}][[1]])
```

```
symGuess= {0.9, 2.9, 4.9, 6.9, 8.9};
```

```
symValues= {nValues[eq5,100,#]
           ,nValues[eq5,200,#]
           ,nValues[eq5,500,#]}&  /@  symGuess;
```

```
asymGuess = {1.9 , 3.9 , 5.9, 7.9 };
```

```
asymValues={nValues[eq6,100,#]
           ,nValues[eq6,200,#]
           ,nValues[eq6,500,#]}& /@  asymGuess;
```

```
(Partition[Sort[{symValues, asymValues} // Flatten], 3] //
  TableForm[#, TableSpacing → {0, 2},
    TableHeadings →
     {{"n=1", "n=2", "n=3", "n=4", "n=5", "n=6", "n=7", "n=8", "n=9"},
      {"V0=100", "V0=200", "V0=500"}}] &)
```

	V0=100	V0=200	V0=500
n=1	0.933848	0.952339	0.969335
n=2	1.86702	1.90442	1.9386
n=3	2.79876	2.85598	2.90773
n=4	3.72819	3.80671	3.87664
n=5	4.65414	4.75628	4.84526
n=6	5.5749	5.70426	5.8135
n=7	6.48773	6.65015	6.78128
n=8	7.38736	7.59322	7.74848
n=9	8.26041	8.53247	8.71498

```
Partition[Sort[{symValues, asymValues} // Flatten], 3] // TableForm[#,
   TableSpacing → {0, 2},
   TableHeadings →
    {{"n=1", "n=2", "n=3", "n=4", "n=5", "n=6", "n=7", "n=8", "n=9"},
     {"V0=100", "V0=200", "V0=500"}}
  ] &
```

	V0=100	V0=200	V0=500
n=1	0.933848	0.952339	0.969335
n=2	1.86702	1.90442	1.9386
n=3	2.79876	2.85598	2.90773
n=4	3.72819	3.80671	3.87664
n=5	4.65414	4.75628	4.84526
n=6	5.5749	5.70426	5.8135
n=7	6.48773	6.65015	6.78128
n=8	7.38736	7.59322	7.74848
n=9	8.26041	8.53247	8.71498

pas 5

```
symRules =
 {kRules, nRule, symSol, a → 1, ℏ → 1, m → 1, V0 → 100, cSym → 100,
   cAsym → 0} // Flatten
```

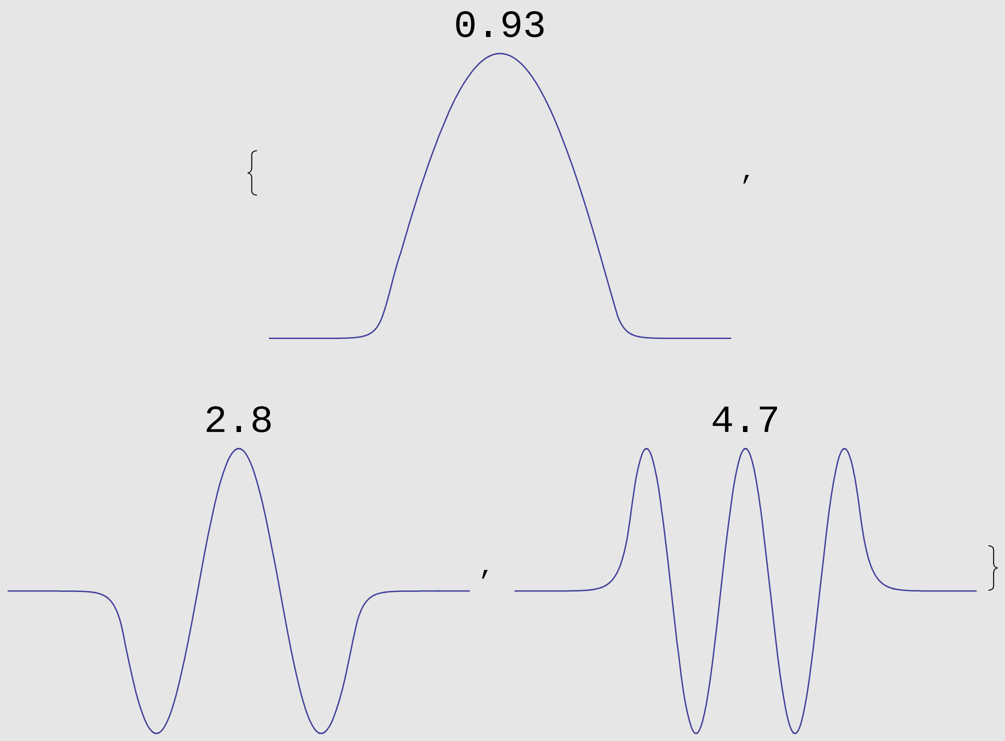
$$\left\{kW \to \frac{\sqrt{2}\ \sqrt{m\ (V0 - Wn)}}{\hbar},\ qLR \to \frac{\sqrt{2}\ \sqrt{m\ Wn}}{\hbar},\ Wn \to V0 - \frac{n^2\ \pi^2\ \hbar^2}{8\ a^2\ m},\right.$$
$$cL \to cSym\ e^{a\ qLR}\ Cos[a\ kW],\ cR \to cSym\ e^{a\ qLR}\ Cos[a\ kW],$$
$$\left. a \to 1,\ \hbar \to 1,\ m \to 1,\ V0 \to 100,\ cSym \to 100,\ cAsym \to 0\right\}$$

```
Clear[sψ,aψ];
(* Symmetric*)
sψ[x_ /;x<-1,n0_]:= (ψL[x]//.symRules//.{n->n0});
sψ[x_ /;-1<=x<1,n0_]:= (ψW[x]//.symRules//.{n->n0});
sψ[x_ /;x>=1,n0_]:= (ψR[x]//.symRules//.{n->n0});
```

```
symEnergy= nValues[eq5, 100,#]&/@symGuess;
```

```
plotsym=
Plot[ sψ[x,#] //.symRules //Evaluate
        ,{x,-2,2}
        ,PlotLabel->  NumberForm[#,2]
        ,Axes->None
        ,DisplayFunction->Identity ]&  /@  symEnergy;
```

```
Show[GraphicsRow[{plotsym[[{1, 2, 3}]], plotsym[[{4, 5}]]}]]
```




```
asymRules =
  {kRules, nRule, asymSol, a → 1, ℏ → 1, m → 1, V0 → 100, cAsym → 100,
    cSym → 0} // Flatten
```

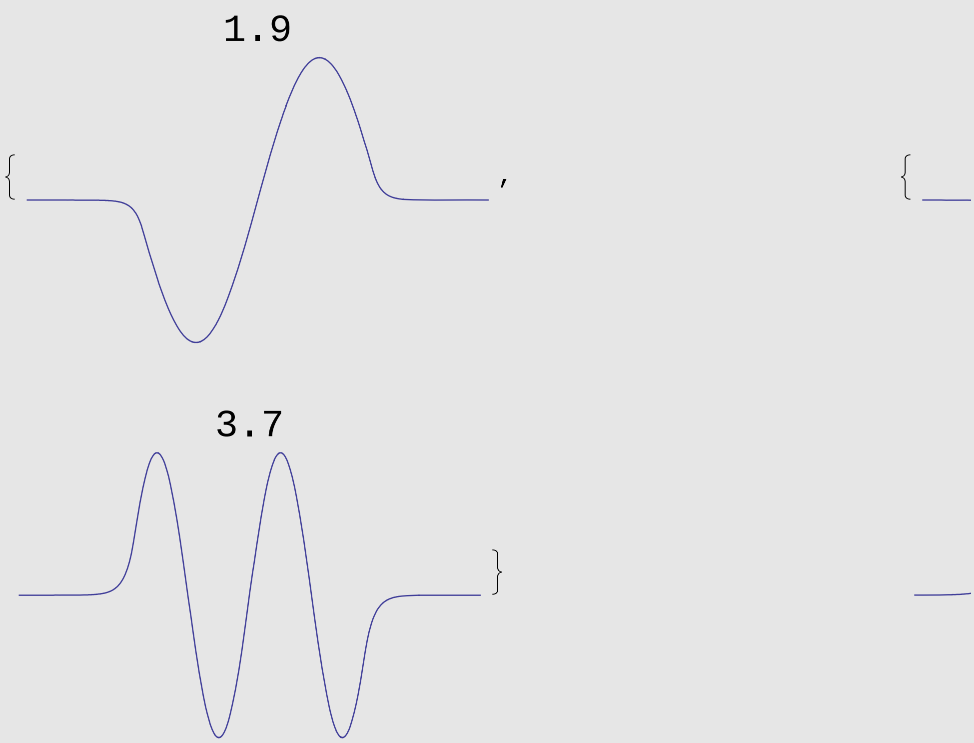
$$\left\{kW \to \frac{\sqrt{2}\,\sqrt{m\,(V0 - Wn)}}{\hbar},\ qLR \to \frac{\sqrt{2}\,\sqrt{m\,Wn}}{\hbar},\ Wn \to V0 - \frac{n^2\,\pi^2\,\hbar^2}{8\,a^2\,m},\right.$$
$$cR \to cAsym\,e^{a\,qLR}\,Sin[a\,kW],\ cL \to -cAsym\,e^{-a\,kW\,Cot[a\,kW]}\,Sin[a\,kW],$$
$$\left. a \to 1,\ \hbar \to 1,\ m \to 1,\ V0 \to 100,\ cAsym \to 100,\ cSym \to 0\right\}$$

```
(* Asymmetric*)
aψ[x_ /;x<-1,n0_]:= (ψL[x]//.asymRules//.{n->n0});
aψ[x_ /; -1<=x<1,n0_]:= (ψW[x]//.asymRules//.{n->n0});
aψ[x_ /;x>=1,n0_]:= (ψR[x]//.asymRules//.{n->n0});
```

```
asymEnergy = nValues[eq6, 100, #] & /@ asymGuess ;
```

```
plotasym=
 Plot[ aψ[x,#] //.asymRules //Evaluate
         ,{x,-2,2}
         ,PlotLabel->NumberForm[#,2]
         ,Axes->None
         ,DisplayFunction->Identity]& /@ asymEnergy;
```

```
Show[GraphicsRow[{plotasym[[{1, 2}]], plotasym[[{3, 4}]]}],
 PlotRange → Automatic]
```



A particle striking a rectangular barrier of width a and height V0.

All calculations are performed in atomic units.

The wavefunctions in the regions 1, 2 and 3

$$\psi_1(x\_) = A\, e^{i\, k\, x} + B\, e^{-i\, k\, x}$$
$$\psi_2(x\_) = C\, e^{i\, k\, x} + D\, e^{-i\, k\, x}$$
$$\psi_3(x\_) = F\, e^{i\, k\, x} + G\, e^{-i\, k\, x}$$

For a particle comming from the left side: G = 0; A value can be choosen 1.

Constants:

In[1]:=
```
Clear["Global`*"];
```

In[2]:=
```
mass  = 931.5;
a     = 10.0;
V0    = 10.0;
hbar  = 197.0;
```

Wave numbers and the discontinuity and propagation matrices:

The probability density.

In[6]:=
```
pd[x_,Ep_] := (

k1 = Sqrt[2*mass*Ep/(hbar^2)];
k2 = Sqrt[2*mass*(Ep - V0)/(hbar^2)];
d12 = 0.5*{ {1 + (k2/k1), 1 - (k2/k1)},
                  {1 - (k2/k1), 1 + (k2/k1)} };
p1 = { {E^(I*k1*a),                0.0},
              {              0.0, E^( -I*k1*a)} };
p2 = { {E^(-I*k2*a),                0},
              {              0.0, E^( I*k2*a)} };
d21 = 0.5*{ {1 + (k1/k2), 1 - (k1/k2)},
                  {1 - (k1/k2), 1 + (k1/k2)} };

(* transfer matrix *)
trans = d12.p2.d21.p1;

(* the amplitudes *)
Aa   = 1.0;
Fa   = Aa/trans[[1,1]];
Ba   = Aa*trans[[2,1]]/trans[[1,1]];
Da = (d12[[1,1]]*Ba - d12[[2,1]]*Aa)/(d12[[1,1]]*d12[[2,2]] - d12[[1,2]]
Ca = (d12[[1,2]]*Ba - d12[[2,2]]*Aa)/(d12[[1,2]]*d12[[2,1]] - d12[[1,1]]
Ga   = 0.0;

(*transmission and reflexion coefficients*)
Ta = 1/(trans[[1,1]]*Conjugate[trans[[1,1]]]);
Ra = trans[[2,1]]*Conjugate[trans[[2,1]]]/(trans[[1,1]]*Conjugate[trans[

(* the wave functions in each region *)
phi1 = Aa*E^( I*k1*x) + Ba*E^(-I*k1*x);
phi2 = Ca*E^( I*k2*x) + Da*E^(-I*k2*x);
phi3 = Fa*E^( I*k1*x) + Ga*E^(-I*k1*x);

(* get the probability density *)
ProbabilityDensity =
     Which[x < 0.0     , phi1*Conjugate[ phi1 ],
            0.0<= x <= a, phi2*Conjugate[ phi2 ],
            a < x,      phi3*Conjugate[ phi3 ]
                ]
 )
```

Plot function

In[7]:=

```
plotf[Ep_] :=
  (plo1 = Plot[pd[x, Ep], {x, -2 a, 2 a}, Frame → True,
     FrameLabel → {"x(fm)", "|ψ\!\(|\^2\)",
       "E=\!\(NumberForm[\(\(Ep, 3\)\)]\) MeV,
         V0=\!\(NumberForm[\(\(V0, 2\)\)]\) MeV,
         a=\!\(NumberForm[\(\(a, 2\)\)]\) fm", " "},
     PlotRange → {{-2 a, 2 a}, {0.`, 1.5` V0}}, RotateLabel → False,
     AxesOrigin → {-2 a, 0}, DisplayFunction → Identity];
   plo3 = ListPlot[{{0, 0}, {0, V0}, {a, V0}, {a, 0}}, Joined → True,
     DisplayFunction → Identity];
   Show[{plo1, plo3}, DisplayFunction → $DisplayFunction]);
```

P2. The probability density for incident proton energy below the potential barrier.

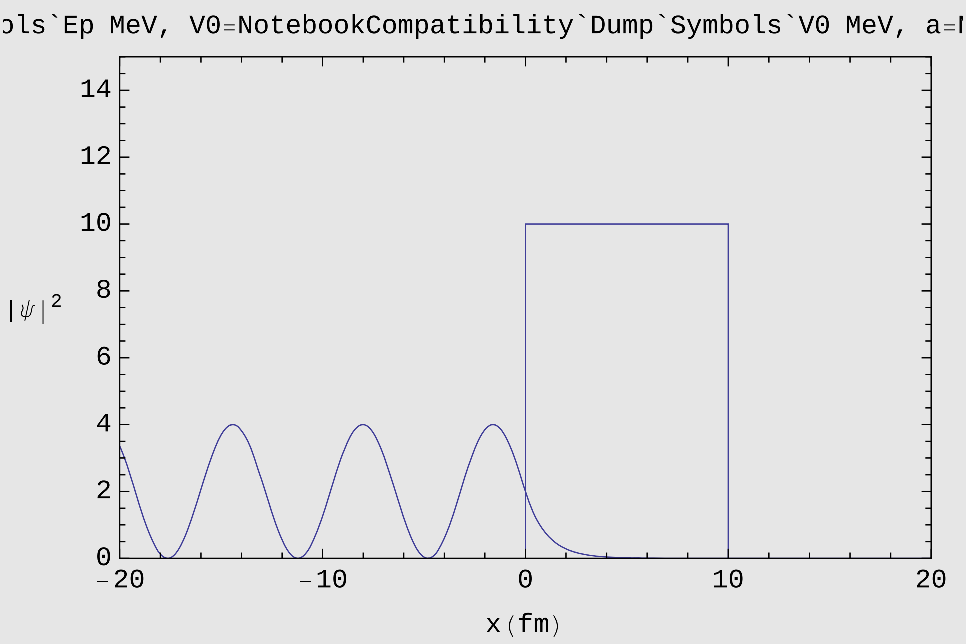
In[8]:=

```
Ep = 0.5 * V0;
```

In[9]:=

```
plotf[Ep]
```

Out[9]=



transmission and reflexion coefficients

In[10]:=

```
Abs[Ta]
```

Out[10]=

```
0.000222137
```

In[11]:=
```
Abs[Ra]
```

Out[11]=
```
0.999778
```

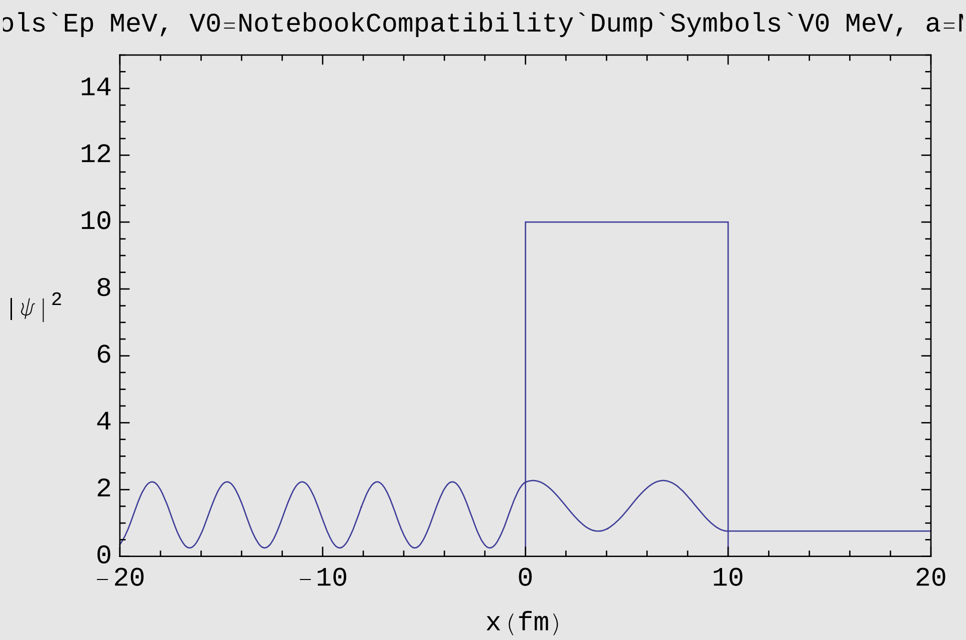
The probability density for incident proton energy above the potential barrier.

In[12]:=
```
Clear[Ep];
```

In[13]:=
```
Ep = 1.5 * V0;
```

In[14]:=
```
plotf[Ep]
```

Out[14]=



transmission and reflexion coefficients

In[15]:=
```
Abs[Ta]
```

Out[15]=
```
0.756524
```

In[16]:=
```
Abs[Ra]
```

Out[16]=
```
0.243476
```

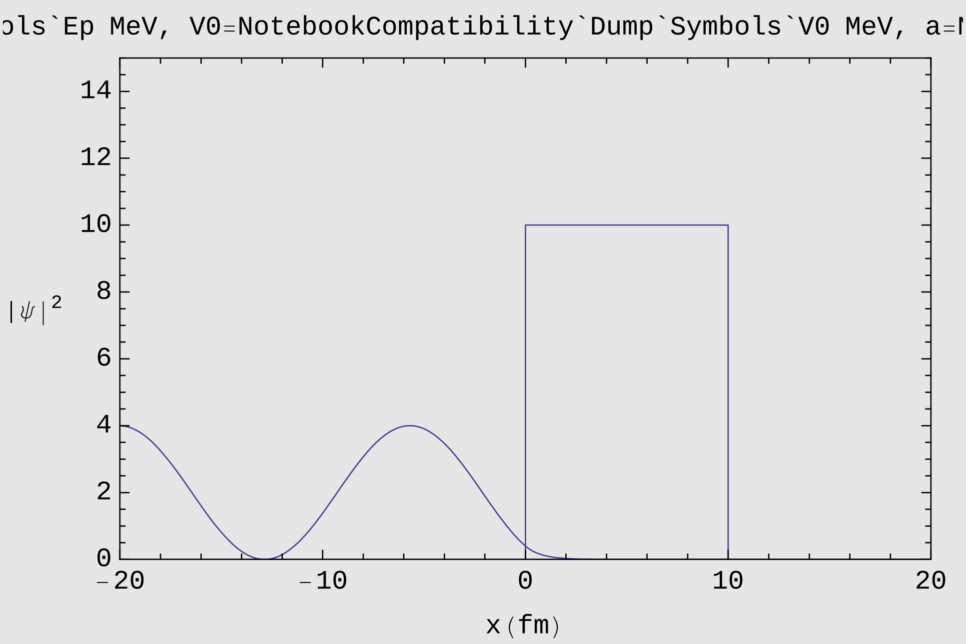
P3. The probability density for energies far less than the barrier height.

In[17]:=
```
Clear[Ep];
```

In[18]:=
```
Ep = 0.1 * V0;
```

In[19]:=
```
plotf[Ep] (*wavelength long because Ep ~ 1/λ*)
```

Out[19]=



In[20]:=
```
Abs[Ta]
```

Out[20]= 2.81291×10^{-6}

In[21]:=
```
Abs[Ra]
```

Out[21]= 0.999997

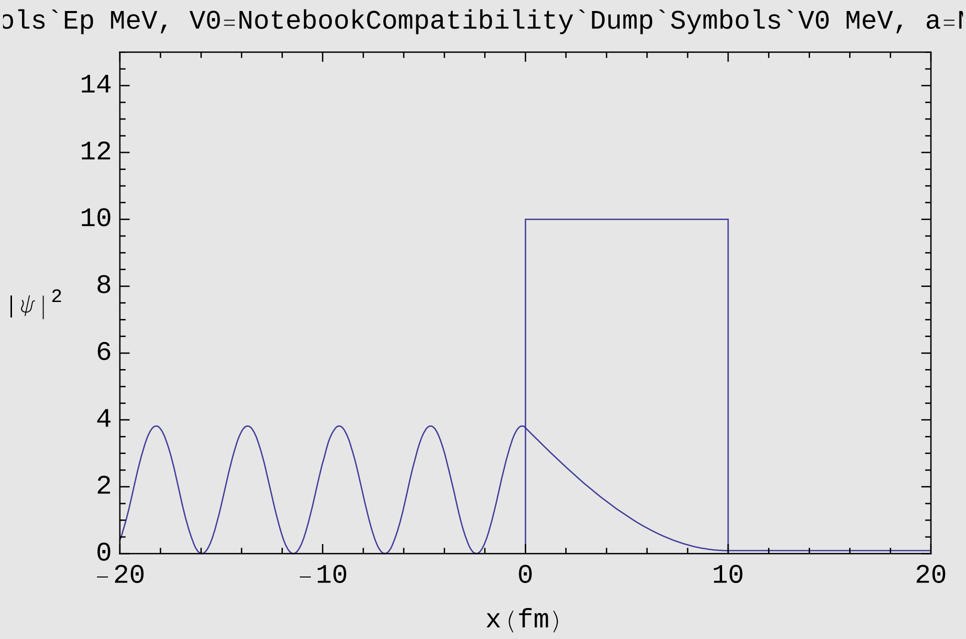
P4. The probability density for energies just above the barrier height.

In[22]:=
```
Clear[Ep];
```

In[23]:=
```
Ep = 1.01 * V0;
```

In[24]:=
```
plotf[Ep]
```

Out[24]=



In[25]:=
```
Abs[Ta]
Abs[Ra]
```

Out[25]= 0.090102

Out[26]= 0.909898

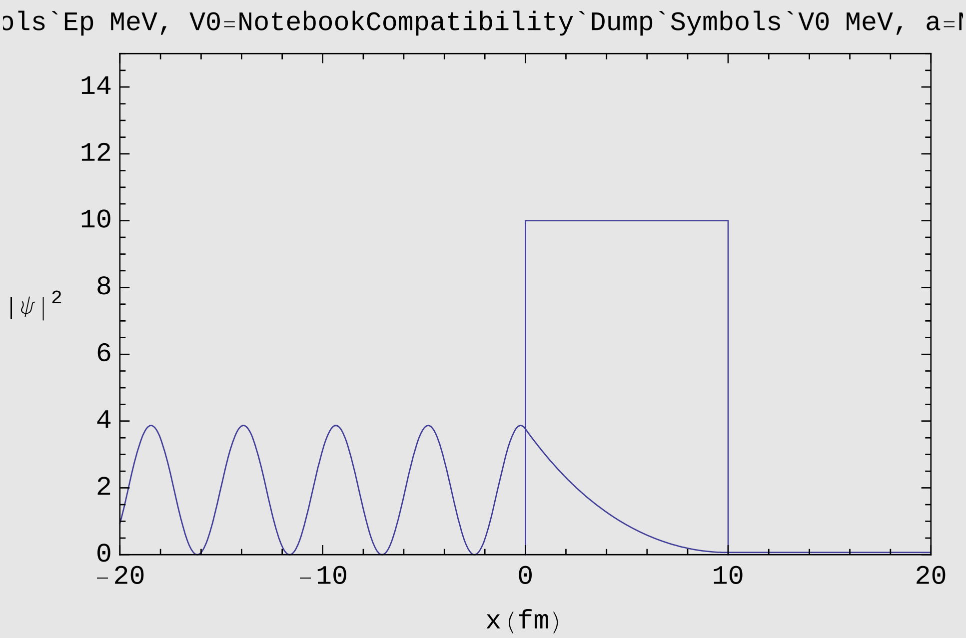
The probability density for energies just below the barrier height.

In[27]:=
```
Clear[Ep];
```

In[28]:=
```
Ep = 0.99 * V0;
```

In[29]:=
```
plotf[Ep]
```

Out[29]=



In[30]:=
```
Abs[Ta]
Abs[Ra]
```

Out[30]= 0.0658304

Out[31]= 0.93417

P5. The beam energy a factor of 3 above the barrier height.

In[32]:=
```
Clear[Ep];
```

In[33]:=
```
Ep = 3 * V0;
```

In[34]:=
```
plotf[Ep];
```

In[35]:=
```
Abs[Ta]
Abs[Ra]
```

Out[35]=
```
0.99448
```

Out[36]=
```
0.00552012
```

P7.Dependence of the transmission coefficient by the energy

In[37]:=
```
Ep =.; Ep = 0.101 * V0; trc = {}; ene = {};
```

In[38]:=
```
While[Ep < 5 * V0,
     plotf[Ep];
      trc = {trc, Abs[Ta]} // Flatten;
      ene = {ene, Ep} // Flatten;
     Ep = Ep + 0.1 * V0;]
```

In[39]:=
```
le = Length[trc];
```

In[40]:=
```
 tranal = {};   (*analytical expression for transmission coeff: p.112,
Messiah*)
```

In[41]:=
```
For[i = 1, i <= le,
 kk = Sqrt[2 * mass * Abs[ene[[i]] - V0] / (hbar^2)];
 tranal =
  {tranal,
    If[ene[[i]] > V0,
      4 * ene[[i]] * Abs[ene[[i]] - V0] /
        (4 * ene[[i]] * Abs[ene[[i]] - V0] +
          V0 * V0 * Sin[kk * a] * Sin[kk * a]),
      4 * ene[[i]] * Abs[ene[[i]] - V0] /
        (4 * ene[[i]] * Abs[ene[[i]] - V0] +
          V0 * V0 * Sinh[kk * a] * Sinh[kk * a])] // Evaluate} // Flatten;
 i++]
```

In[42]:=
```
(*l1: calculated transmission coeff : points;
l2 - analytical expression: line*)
l1 = ListPlot[Table[{ene[[i]], trc[[i]]}, {i, 1, le}],
   DisplayFunction → Identity, PlotStyle → PointSize[0.02`]];
l2 = ListPlot[Table[{ene[[i]], tranal[[i]]}, {i, 1, le}], Joined → True,
   DisplayFunction → Identity];
re = Show[{l1, l2}, DisplayFunction → $DisplayFunction]
```

Out[44]=