

$$i \frac{\partial \Psi(x, t)}{\partial t} = -\frac{1}{2} \frac{\partial^2 \Psi(x, t)}{\partial x^2} + V(x) \Psi(x, t)$$

$$\Psi(-x_M, t) = \Psi(x_M, t) = 0.$$

In[314]:=

```
xM = 100;
W = 17;
schrodingerEq =
ID[Ψ[x, t], {t, 1}] == -1/2 D[Ψ[x, t], {x, 2}] + W UnitBox[(x - 3)] Ψ[x, t]
```

Out[316]= $i \Psi^{(0,1)}[x, t] == 17 \text{UnitBox}[-3 + x] \Psi[x, t] - \frac{1}{2} \Psi^{(2,0)}[x, t]$

```
In[4]:= enforceDirichletBCs[ψ_, x_, xM_] :=
ψ - ((- (ψ /. x -> xM) + (ψ /. x -> -xM))) / 2 *
(Cos[(x + xM) / (2 xM) Pi] + 1) + (ψ /. x -> xM)
```

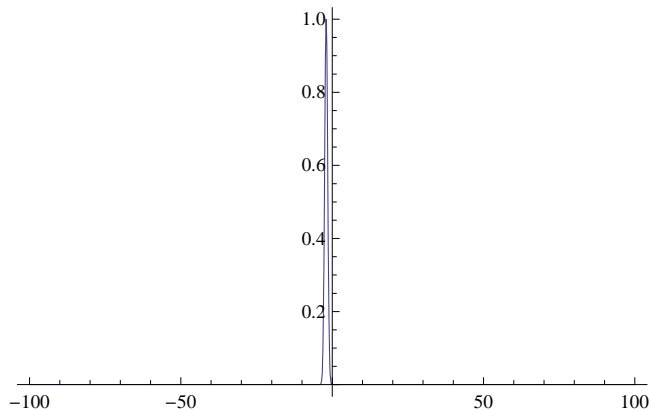
```
In[317]:= myψ[x_] = enforceDirichletBCs[Exp[-(x + 2)^2] Exp[5 I x], x, xM] // Chop[#, 10^-6] &
Chop[With[{ψ = myψ[x]},
-1/2 NIntegrate[Evaluate[D[ψ, {x, 2}] Conjugate[ψ]],
{x, -xM, xM}, MinRecursion -> 50, MaxRecursion -> 50]], 10^-3]
```

Out[317]= $-e^{-10404+500 i} + e^{5 i x-(2+x)^2} - \frac{1}{2} (-e^{-10404+500 i} + e^{-9604-500 i}) \left(1 + \text{Cos}\left[\frac{1}{200} \pi (100 + x)\right] \right)$

Out[318]= 16.2931

```
In[293]:= Plot[Abs[myψ[x]]^2, {x, -xM, xM}, PlotRange -> All]
```

Out[293]=



In[319]:= nsol =

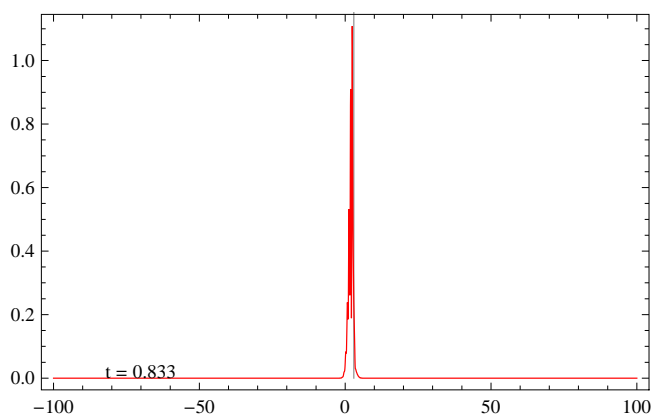
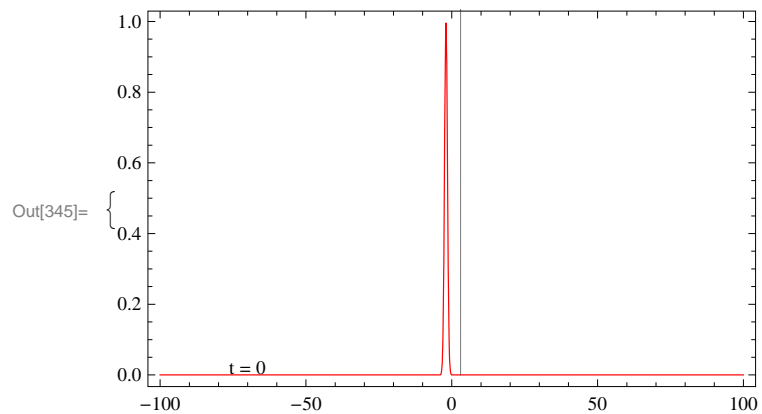
```
NDSolve[{schrodingerEq,
Ψ[x, 0] == myψ[x], Ψ[xM, t] == 0, Ψ[-xM, t] == 0}, Ψ, {x, -xM, xM}, {t, 0, 10},
AccuracyGoal -> 2, PrecisionGoal -> 2, MaxSteps -> 500, Method -> {"MethodOfLines",
"SpatialDiscretization" -> {"TensorProductGrid", "MinPoints" -> {600}}];
```

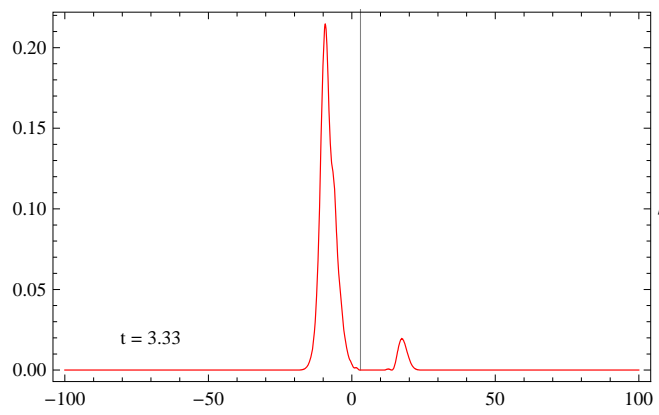
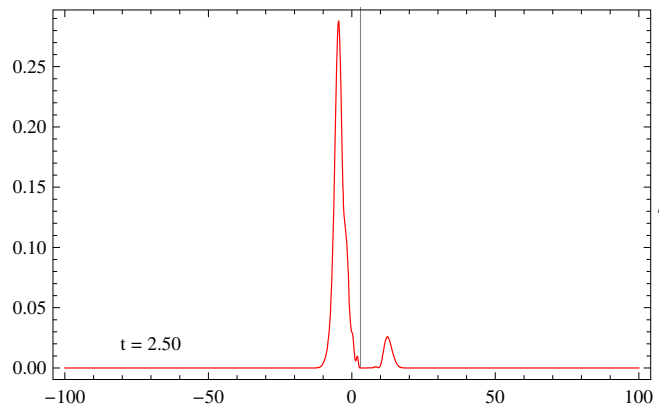
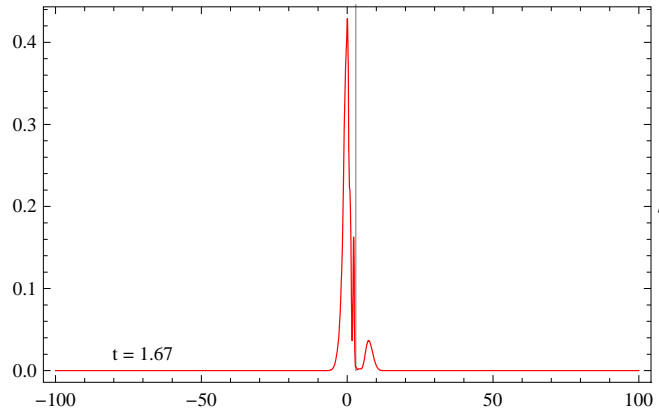
```
In[306]:= DensityPlot[Evaluate[Abs[Ψ[x, t]]^2 /. nsol[[1]]],
{x, -xM, xM}, {t, 0, 10}, PlotPoints -> 200, Mesh -> False,
ColorFunction -> (Hue[0.78 #] &),
Epilog -> {Thick, GrayLevel[0], Line[{{0.5, 0}, {0.5, 10}], Line[{{5.5, 0}, {5.5, 10}}]}]
```

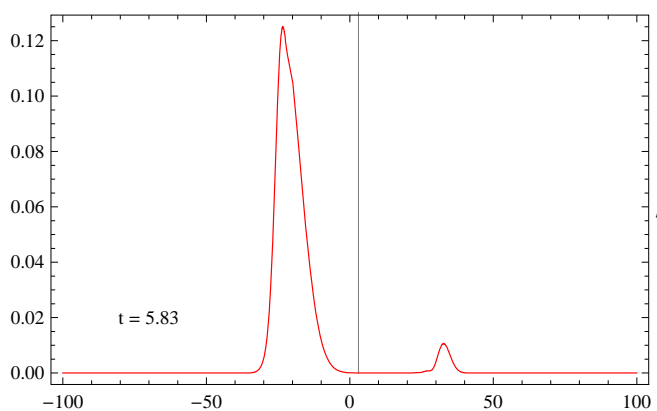
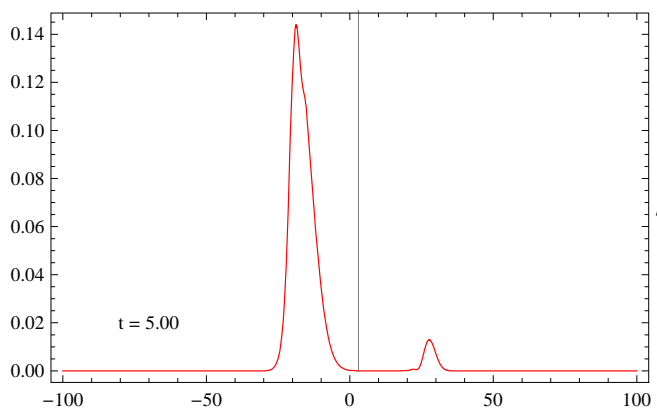
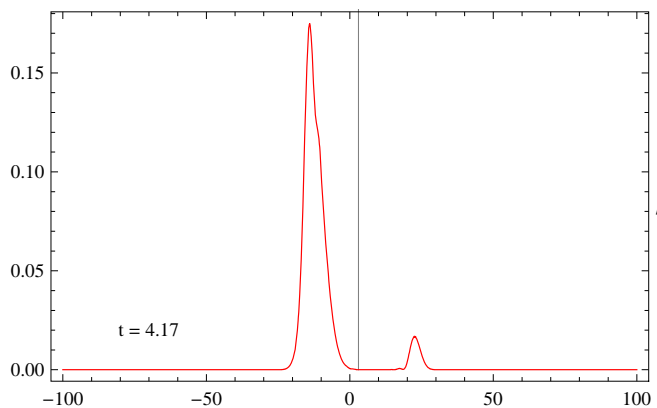
Out[306]= \$Aborted

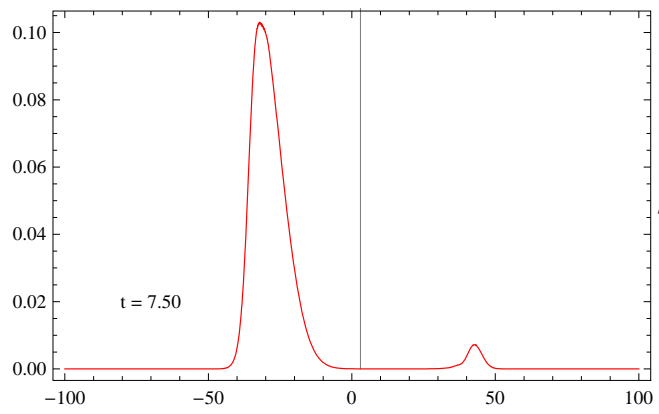
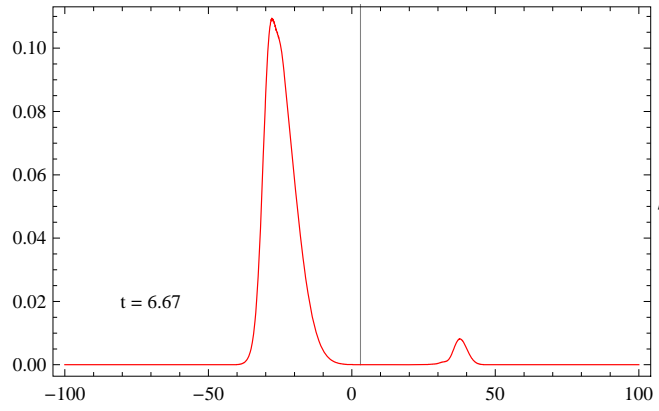
$|\psi(x,t)|^2$

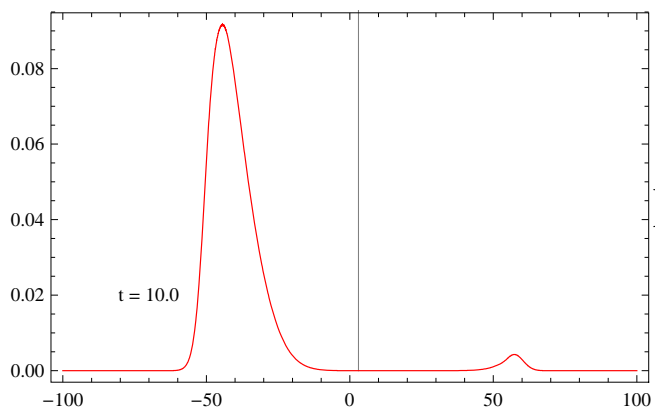
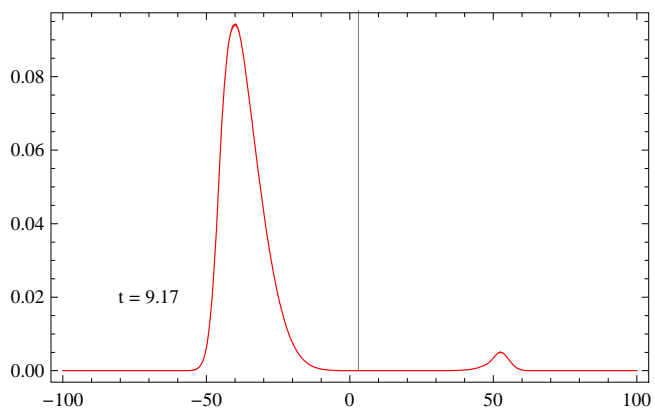
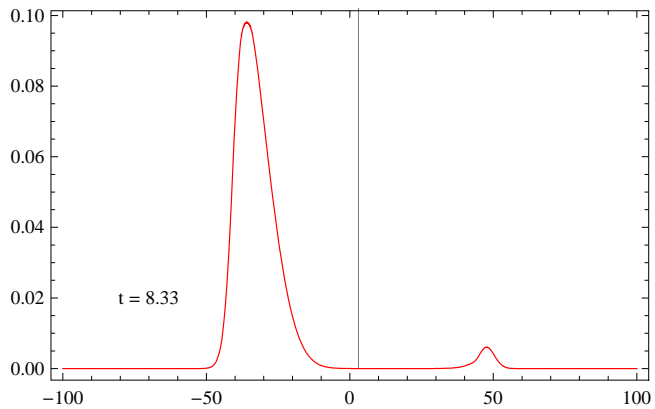
```
In[345]:= Table[Plot[Evaluate[Abs[Ψ[x, t]]^2 /. nsol], {x, -xM, xM},  
  PlotRange -> All, Prolog -> {GrayLevel[0.5], Line[{{3, 0}, {3, 1.5}}]},  
  Frame -> True, Axes -> False, PlotStyle -> {{Hue[0], Thickness[0.002]}},  
  Epilog -> {GrayLevel[0], Text["t = " <> ToString[N[t, 3]], {-70, 0.02}}],  
  {t, 0, 10, 10/12}]
```





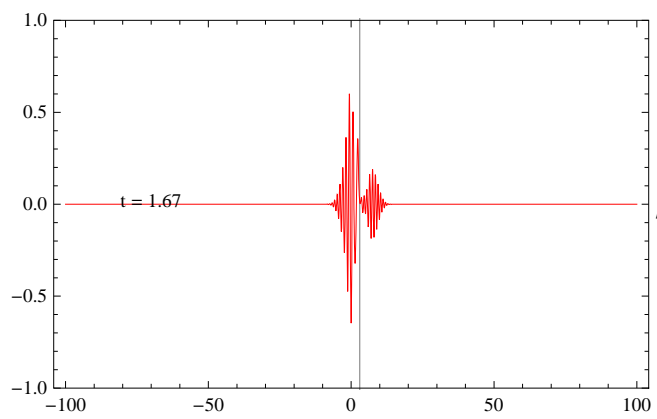
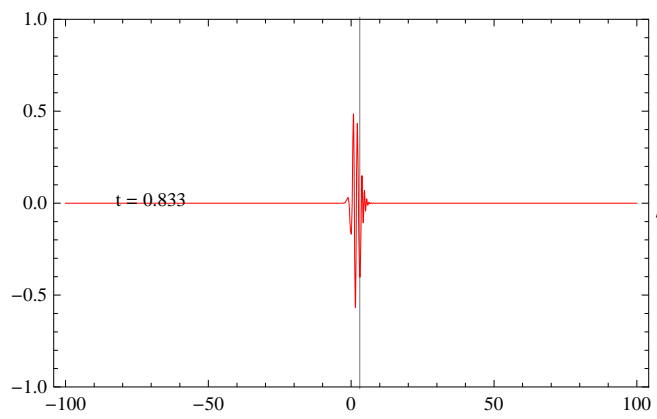
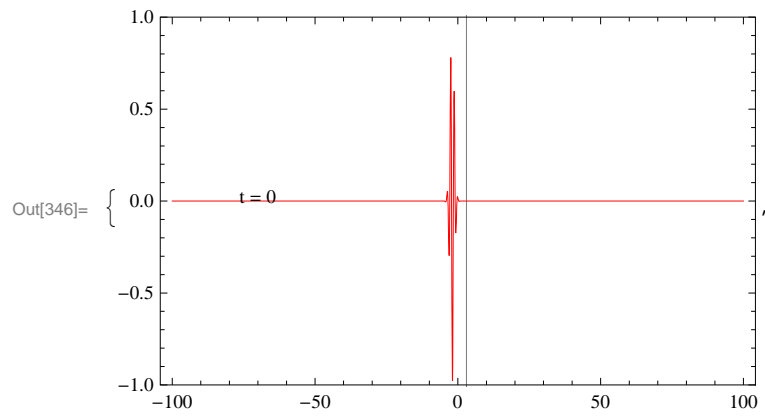


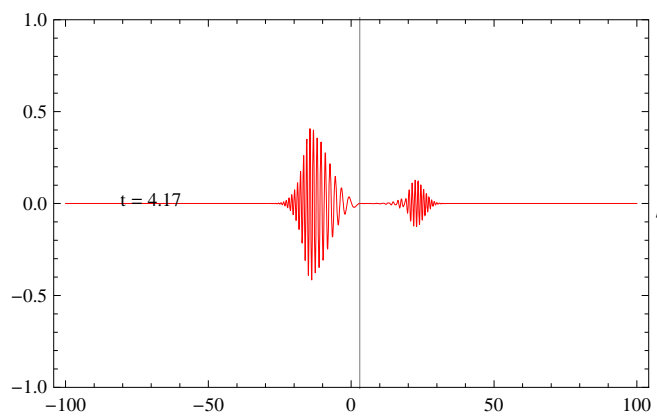
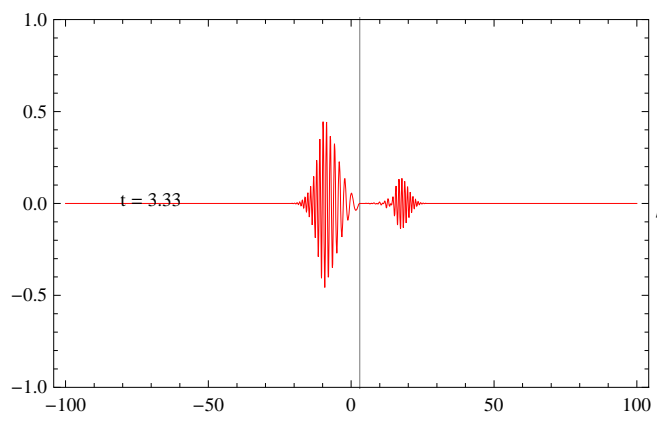
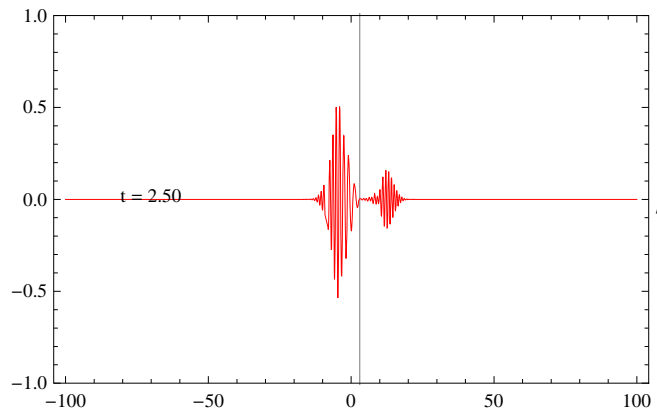


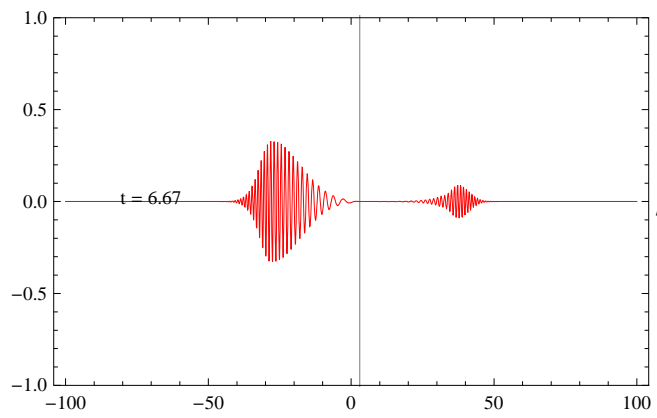
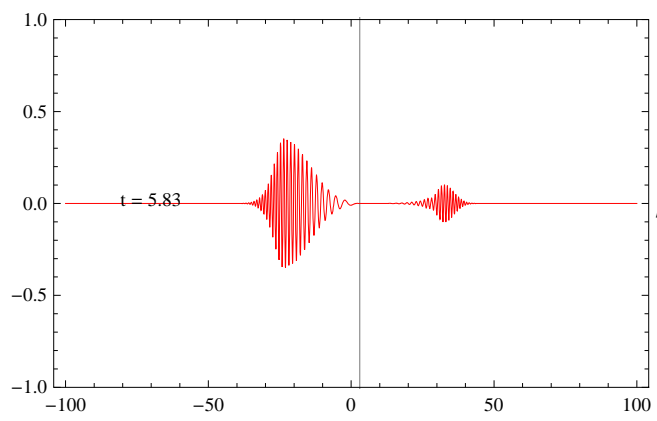
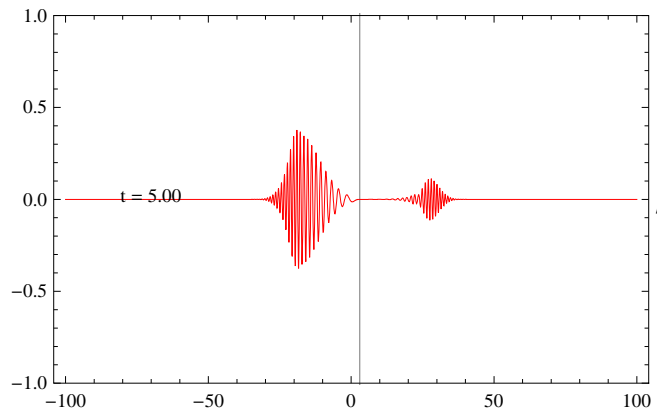


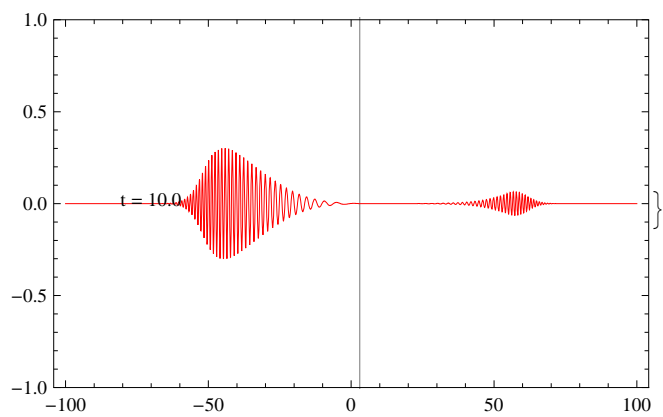
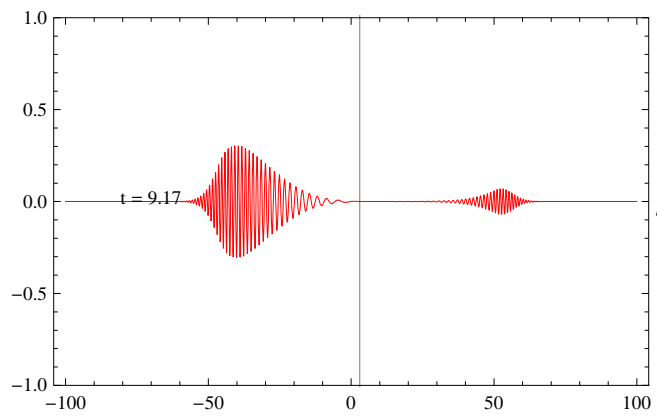
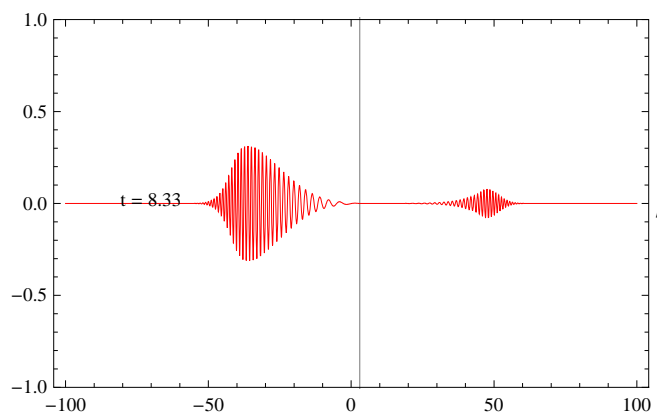
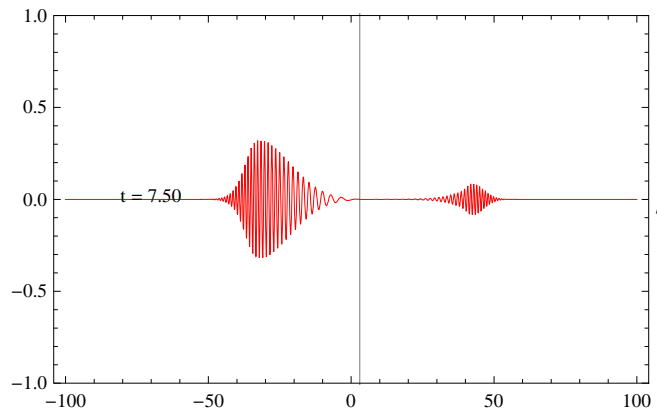
Re($\psi(x,t)$)

```
In[346]:= Table[Plot[Evaluate[Re[Ψ[x, t]] /. nsol], {x, -xM, xM},
  PlotRange -> {-1, 1}, Prolog -> {GrayLevel[0.5], Line[{{3, -2}, {3, 2}}]},
  Frame -> True, Axes -> False, PlotStyle -> {{Hue[0], Thickness[0.001]}},
  Epilog -> {GrayLevel[0], Text["t = " <> ToString[N[t, 3]], {-70, 0.02}]},
  {t, 0, 10, 10/12}]
```



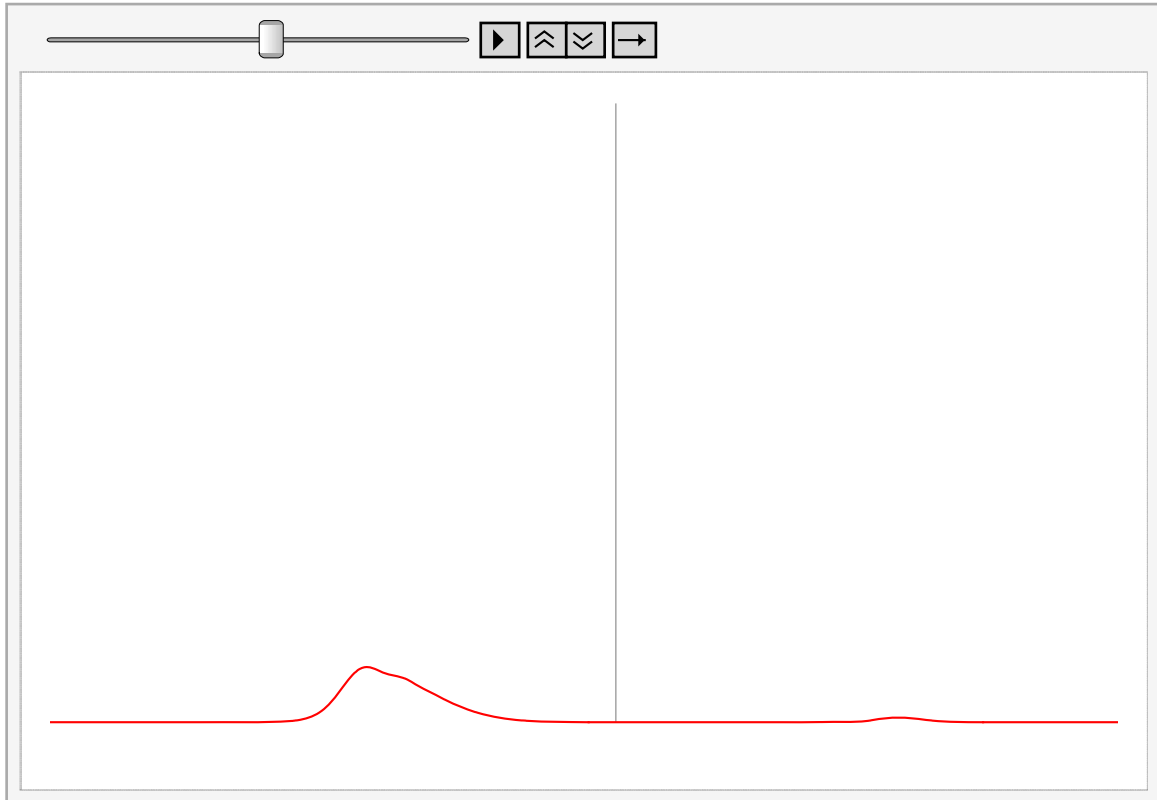




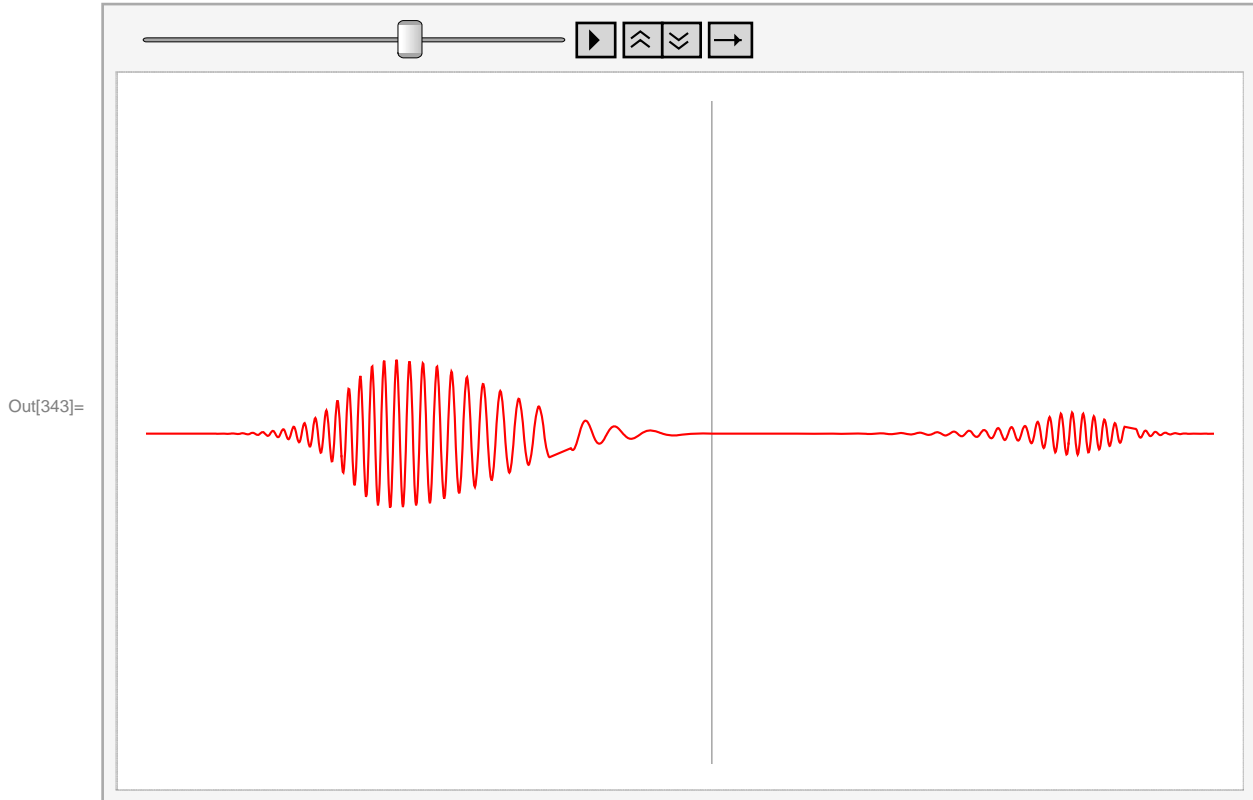


```
In[340]:= ListAnimate[Table[Plot[Evaluate[Abs[Ψ[x, t]]^2 /. nsol],  
  {x, -xM, xM}, PlotRange -> {{-50, 50}, {-0.1, 1.5}},  
  Prolog -> {GrayLevel[0.5], Line[{{3, 0}, {3, 1.5}}]}, Frame -> False,  
  Axes -> False, PlotStyle -> {{Hue[0], Thickness[0.002]}}, Epilog ->  
  {GrayLevel[0], Text["t = " <> ToString[N[t, 3]], {-10, 4}], ImageSize -> 500},  
  {t, 0, 10, 10/100}], 15, AnimationRunning -> False]
```

Out[340]=



```
In[343]:= ListAnimate[Table[Plot[Evaluate[Re[Ψ[x, t]] /. nsol],
  {x, -xM, xM}, PlotRange -> {{-50, 50}, {-1.5, 1.5}},
  Prolog -> {GrayLevel[0.5], Line[{{3, -2}, {3, 2}}]}, Frame -> False,
  Axes -> False, PlotStyle -> {{Hue[0], Thickness[0.002]}}, Epilog ->
  {GrayLevel[0], Text["t = " <> ToString[N[t, 3]], {-10, 4}], ImageSize -> 500},
  {t, 0, 10, 10/100}], 15, AnimationRunning -> False]
```



```
Export["electron2.gif",
  ListAnimate[Table[Plot[Evaluate[Abs[Ψ[x, t]]^2 /. nsol], {x, -xM, xM}, PlotRange ->
    {{-50, 50}, {-0.1, 1.5}}, Prolog -> {GrayLevel[0.5], Line[{{3, 0}, {3, 1.5}}]},
    Frame -> False, Axes -> False, PlotStyle -> {{Hue[0], Thickness[0.002]}}, Epilog ->
    {GrayLevel[0], Text["t = " <> ToString[N[t, 3]], {-10, 4}], ImageSize -> 500},
    {t, 0, 10, 10/100}], 15]]
```

Export::infer : Cannot infer format of file electron2.mov. >>

Out[347]= \$Failed

```
In[348]:= momentum[t_, n_] :=
  With[{f = Ψ /. nsol[[1]]},
    Fourier[Table[f[x, t], {x, -xM, xM, 2 xM / n}]]]
```

```
In[349]:= ListPlot3D[Abs[Table[momentum[t, 100], {t, 0, 10, 10/100}]],  
  Mesh -> False, AxesLabel -> {p, t}]
```

