Causal Wave Packet Spreading

Sharp Questions and Answers

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The non-relativistic Schrödinger equation gives wave packets that spread infinitely fast, in the sense that even if they start out in a confined region, they extend over all space immediately afterward.

Related to this, there are issues around “time under the barrier” in tunneling problems that have been debated, inconclusively, for many years.

Given advances in precision trapping and sudden releasing of particles, and in resolving short time intervals - broadly, “attosecond physics” - the problem getting a clear, quantitative account of wave packet spreading that does a better job of respecting special relativity seems timely.

(1) Refining Uncertainty

Limits of Localization

To pose questions around superluminal spreading - that is, presumably, its absence, and the existence or not of *near*-luminal spreading - sharply, one should start with wave functions that are strictly localized in space.

On the other hand it is desirable to suppress, or at least keep watch over, the large-k and high-energy components, since these are going to bring in high velocities (and, in tunneling, over-the-barrier propagation) “trivially”.

These requirements are in tension, for reasons related to the uncertainty principle. But here the uncertainty principle as such is too crude for our purposes.

It is relatively simple to show that one cannot have strict limits in both position and momentum space.

(Proof: The Fourier transform of a function that is bounded in space can be continued into an analytic function in a strip around the real axis. But the only analytic function that vanishes in an interval is just plain zero.)

There is a remarkable theorem that tells a precise, detailed story:

3. The Beurling-Malliavin theorem

I will conclude the note by stating a difficult result in harmonic analysis which fully answers the question you asked. It gives the conditions for a function $\omega(\xi)$ under which one can construct a compactly supported function f satisfying

$$|\hat{f}(\xi)| \leq \omega(\xi) \tag{3.1}$$

Note that this is very strong because you can actually ask ω to be non-monotone, so you could for example ask $\hat{f}$ to be very small on specific intervals but have otherwise relatively slow decay.

There are two conditions:

- **Log-integrability**: We must have $0 < \omega \leq 1$ and

$$\int \frac{\log \omega(\xi)}{1+\xi^2} \, \mathrm{d}\xi > -\infty. \tag{3.2}$$

- **Lipschitz regularity**: For some $K > 0$ it holds that for every $\xi, \eta \in \mathbf{R}$

$$|\log(\xi) - \log(\eta)| \leq K|\xi - \eta|. \tag{3.3}$$

Should be $\log \omega(\xi)$ etc .

The integrability for example means that you cannot take $\omega(\xi) = \exp(-|\xi|)$ since $\int \frac{-|\xi|}{1+|\xi|^2} \, \mathrm{d}\xi$ does not converge. On the other hand $\omega(\xi) = \exp(-|\xi|/\log(|\xi|^2))$ is fine because $\int \frac{-|\xi|}{(1+|\xi|^2)(\log^2(|\xi|))} \, \mathrm{d}\xi$ does converge.

The Lifshitz condition

tell you that if ω is going to be very small at some point it actually has to be small near that point too. look like exponential growth or decay.

Theorem 3.1 (Beurling-Malliavin). *If ω satisfies log-integrability and Lipschitz regularity as above, then there exists a nonzero f with* $\operatorname{supp} f \subset [-1, 1]$ *such that*

$$|\hat{f}(\xi)| \leq \omega(\xi). \tag{3.4}$$

Special thanks to Felipe Hernandez

There are good practical constructions based on the following classic function that is **smooth (but not analytic)** and vanishes on one side:

$$f(x) \ = \ H(x)\, e^{-\frac{1}{x}}$$

Its Fourier transform falls off as

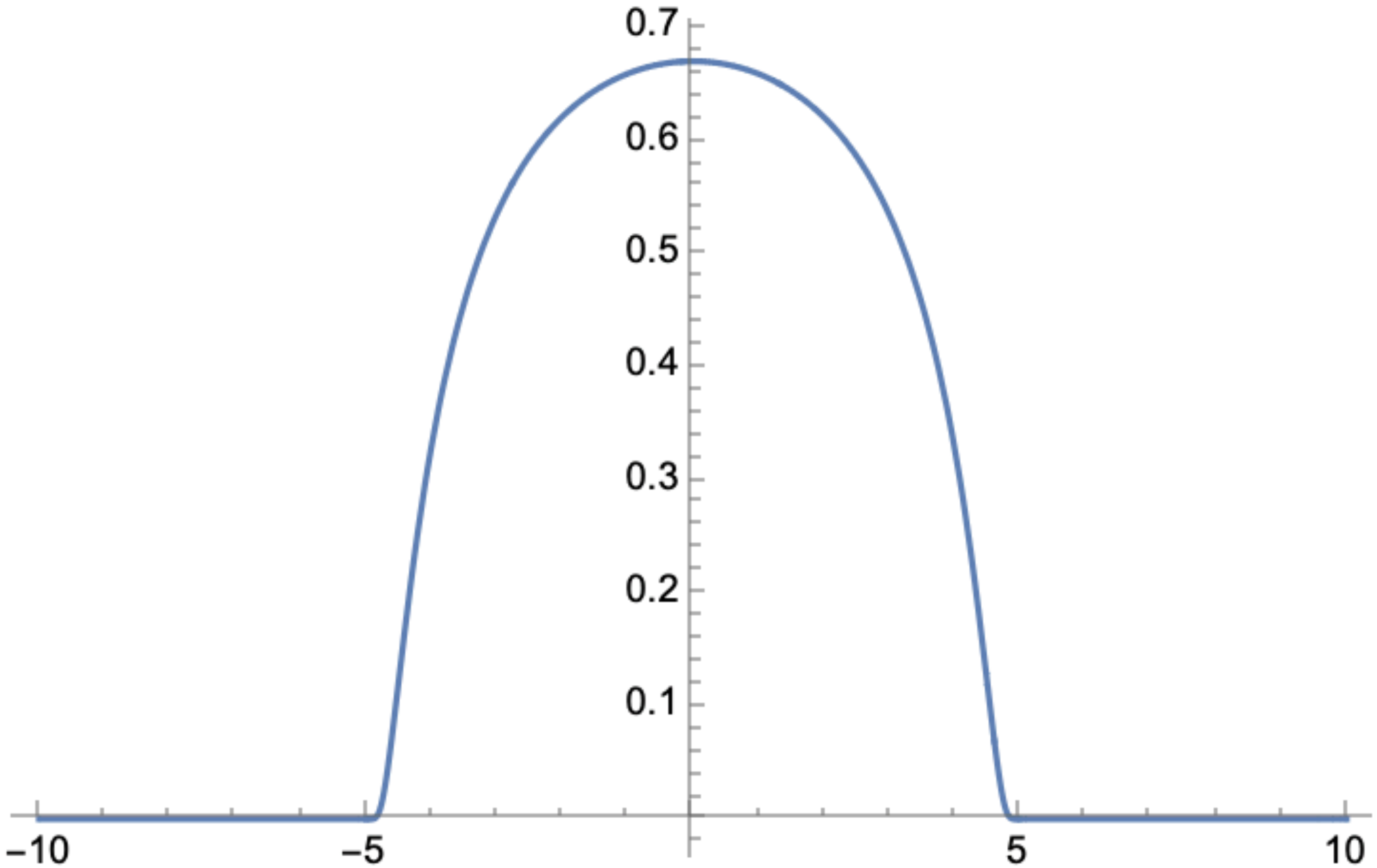
$$\int e^{ikx} f(x) \ \sim \ e^{i\sqrt{2k}} e^{-\sqrt{2k}}$$

Multiplying by a translated reflection, we get a nice windowing function:

In[•]:=
```
smoothBox[a_, x_] := smoothieLeftZero[a - x] * smoothieLeftZero[a + x]
```

In[•]:=
```
Plot[smoothBox[5, x], {x, -10, 10}]
```

Out[•]=

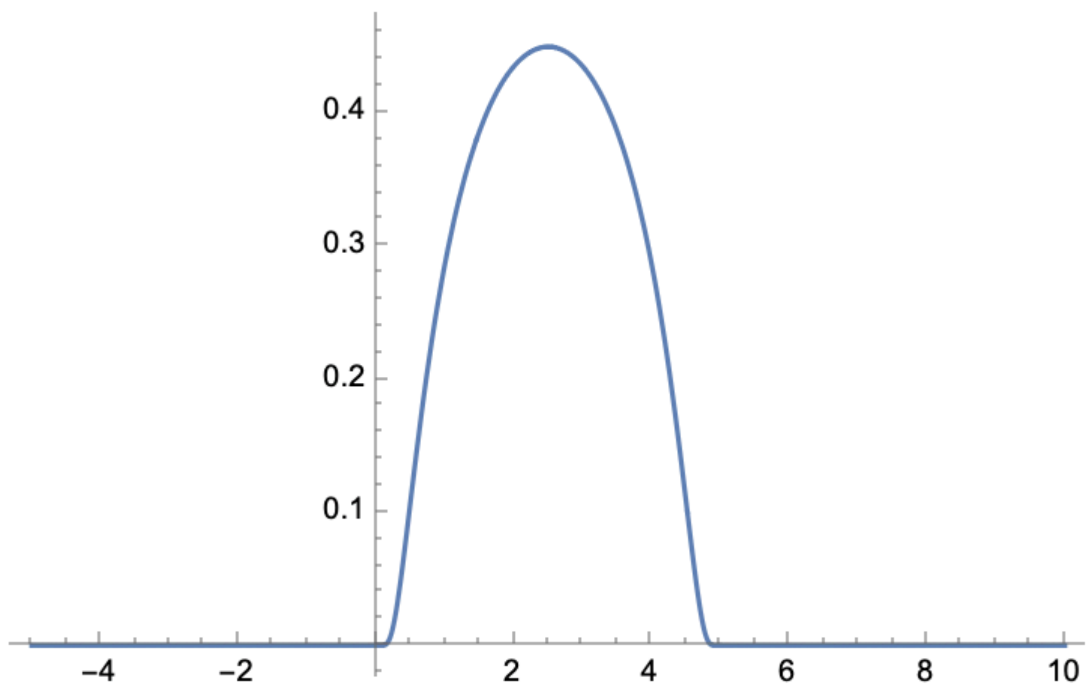


```
In[∘]:= smoothieLeftZero[x_] := Piecewise[{{0, x ≤ 0}, {Exp[-1 / x], x > 0}}]

In[∘]:= g[x_] := smoothieLeftZero[x] * smoothieLeftZero[5 - x]

In[∘]:= Plot[g[x], {x, -5, 10}]
```

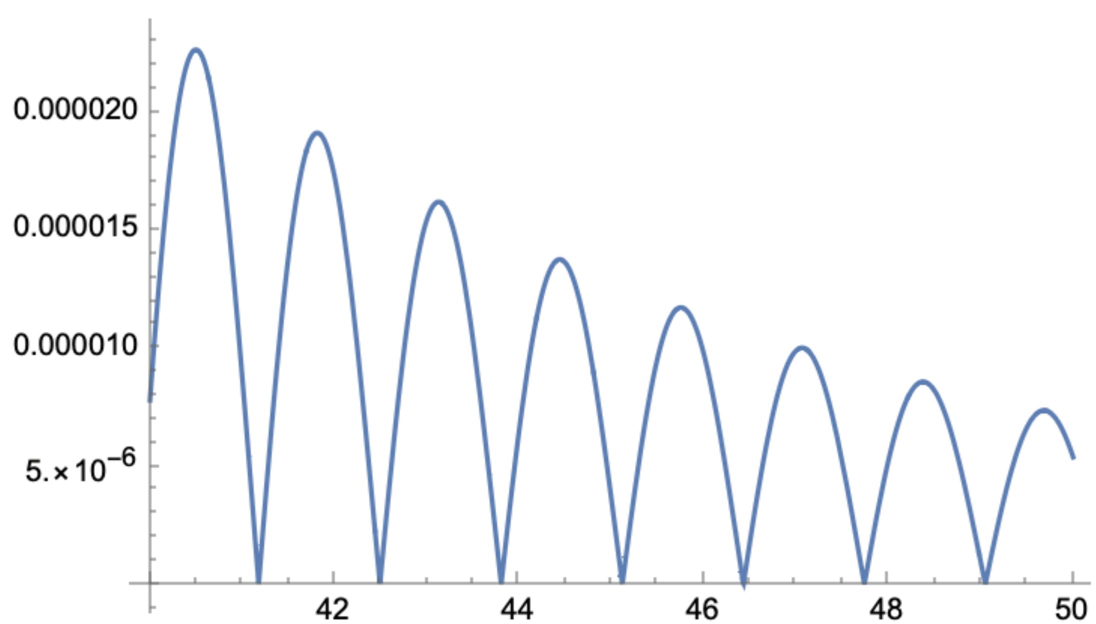
Out[∘]=




```
In[∘]:= h[k_] := NIntegrate[Exp[k * I * x] * g[x], {x, -1, 6}]

In[∘]:= Plot[Abs[h[k]], {k, 40, 50}]
```

Out[∘]=



To have more flexibility, we could consider

$$h(c, \alpha, x) = 0\,;\; x \leq 0$$

$$h(c, \alpha, x) = \exp\left(-c/x^{\alpha}\right);\; x > 0$$

which leads to

$$\int e^{ikx}\, h(c, \alpha, x) \;\sim\; \exp\left(-k^{\frac{\alpha}{\alpha+1}}\,(\alpha+1)\,(\alpha c)^{\frac{1}{\alpha+1}}\,(\sin\frac{\pi}{2(\alpha+1)} \;-\; i\cos\frac{\pi}{2(\alpha+1)})\right)$$

(2) Restoring Relativity

Schrödinger to Klein-Gordon

Now let's put a causal equation - namely, (complex) Klein-Gordon - underneath the spinless Schrödinger equation.

Mathematically, this is not difficult:

$$\partial_t^2\phi - \partial_x^2\phi + m^2\phi = 0$$

$$\phi = e^{-imt}\psi$$

$$-2im\partial_t\psi + \partial_t^2\psi - \partial_x^2\psi = 0$$

Conceptual issues:

- What is the conserved density?
- What is the initial value problem?
- What is causality? (Already addressed.)
- What are we talking about?

Conserved Current

$$j_\mu \;=\; \mathrm{Im}\,\phi^* \partial_\mu \phi$$

$$j_0 \to -m\psi^\dagger\psi + \mathrm{Im}\,\psi^*\partial_0\psi \approx -m\psi^* + \frac{1}{4m}(\nabla^2\psi^*\psi + \psi^*\nabla^2\psi)$$

Thus, $\psi^*\psi - \frac{1}{4m^2}\nabla\psi^*\nabla\psi$ is a more accurate representation of charge density than $\psi^*\psi$. Of course, it is has the appropriate large m limit.

It is not positive definite, but unless the NR Schrödinger equation is being misapplied regions of negativity will be small, and impossible to resolve without bringing in large momenta.

“Self-Consistent” Initial Value Problem

Since the KG equation is second order, we need the time derivative of the initial wave function as well as the wave function itself.

A nice way to finesse this issue is to impose the NR Schrödinger equation at time 0.

Role of PDEs in QFT

They govern appropriate correlation functions.

The correlation functions, in turn, govern physical excitation and detection processes. Glauber spelled this out in the context of QED and photo-detection.

(3) Comparing Green Functions

Correspondence and Divergence

Non-relativistic Propagator (Green Function)

$$\psi(x,t) \;=\; \int dx\, G(x-x',t-t')\,\psi(x',t')$$

$$G_{sNR}(x,t;0,0) \;=\; \sqrt{\frac{m}{2\pi i t}}\exp\frac{imx^2}{2t}$$

Relativistic Green Function(s)

$$\phi(x,0) \;=\; f(x) \qquad \partial_t\phi(x,0) \;=\; g(x) \quad (\partial_t^2 - \partial_x^2 + V(x))\phi(x,t) \;=\; 0$$

$$\phi(x,t) \;=\; \int dx' G^\sigma(x,t;x',0)f(x') + \int dx' G^\tau(x,t;x',0)g(x')$$

$$(\partial_t^2 - \partial_x^2 + m^2)G^\sigma(x,t;x',t') \;=\; 0$$

Even in $t - t'$

$$\partial_t G^\sigma(x,t;x',t) \;=\; 0 \qquad G^\sigma(x,t;x',t) \;=\; \delta(x-x')$$

$$(\partial_t^2 - \partial_x^2 + m^2)G^\tau(x,t;x',t') \;=\; 0$$

Odd in $t - t'$

$$G^\tau(x,t;x',0) \;=\; 0 \qquad \partial_t G^\tau(x,t;x',0) \;=\; \delta(x-x')$$

$$G^{\tau}(x, t; 0,0) = \frac{1}{2}\left(H(x+t) - H(x-t)\right) J_0(m\tau)$$

$$(\tau = \sqrt{t^2 - x^2})$$

$$G^{\sigma}(x, t; 0,0) \ = \ \frac{\partial}{\partial t} G^{\tau}(x, t; 0,0)$$

Non-Relativistic Limit of Relativistic Green Function

$$e^{-imt}\psi(x,t) \;\approx\; \int dx' G^{\sigma}(x,t;x',0)\psi(x',0) - im\int dx' G^{\tau}(x,t;x',0)\psi(x',0)$$

$$= \;\int dx'(\partial_t - im)G^{\tau}(x,t;,x',0)\psi(x',0)$$

$$G_{\mathrm{cNR}}(x,t;x',0) \;=\; e^{imt}(\partial_t - im + \frac{i}{2m}\partial_x^2)\,G^{\tau}(x,t;x',0)$$

Incorporating "self-consistency";
applicable to ψ

(Pictorial) Numerical Comparisons: Correspondence and Divergence

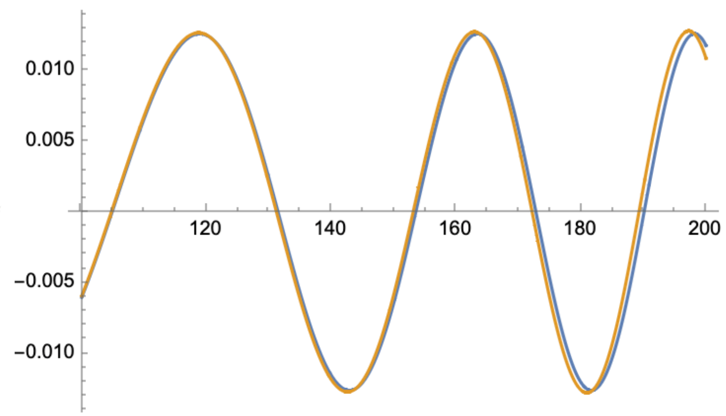
$m = 1$

Real parts

```
In[∘]:= Plot[{Re[greenSNR[x, 1000]], Re[greenIMP0[x, 1000]]}, {x, 100, 200}, PlotRange → All, PlotPoints → 1000]
```

0.01 →

Out[∘]=

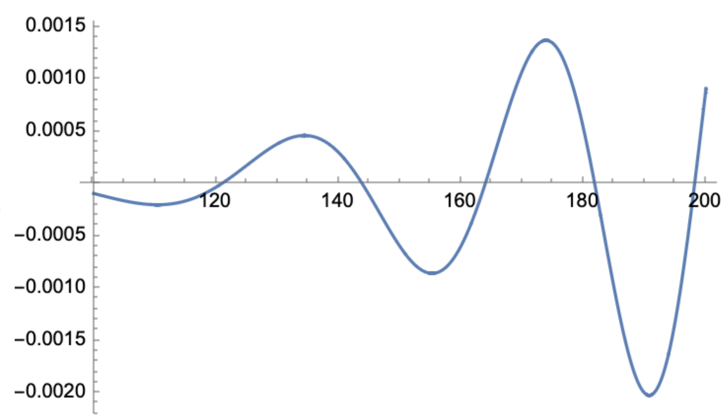


t = 1000, 0 < x < 100;
overlay

```
In[∘]:= Plot[Re[greenSNR[x, 1000]] - Re[greenIMP0[x, 1000]], {x, 100, 200}, PlotRange → All, PlotPoints → 1000]
```

0.0015 →

Out[∘]=

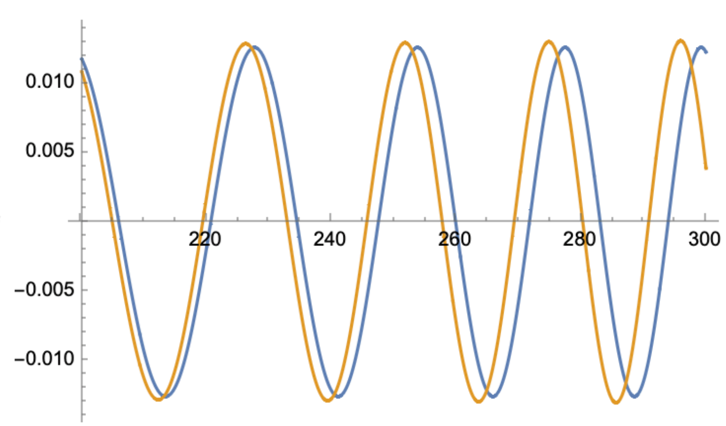


t = 1000, 0 < x < 100;
absolute difference

```
In[∘]:= (*blue plotted first*)
In[∘]:= Plot[{Re[greenSNR[x, 1000]], Re[greenIMP0[x, 1000]]}, {x, 200, 300}, PlotRange → All, PlotPoints → 1000]
```

0.01 →

Out[∘]=

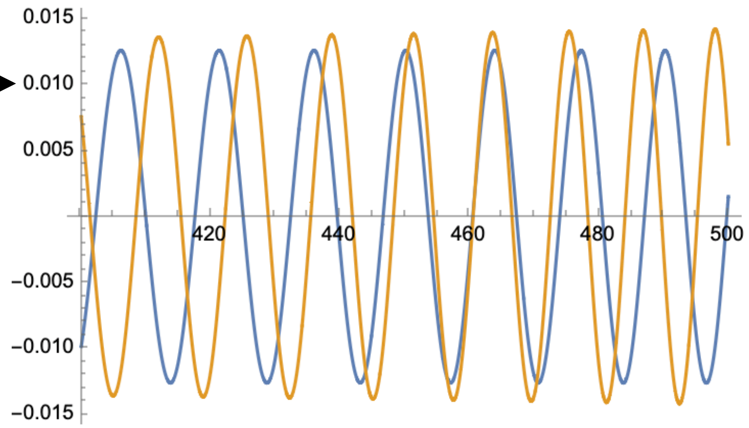


t = 1000, 200 < x < 300;
overlay

```
In[∘]:= Plot[{Re[greenSNR[x, 1000]], Re[greenIMP0[x, 1000]]}, {x, 400, 500}, PlotRange → All, PlotPoints → 1000]
```

0.01

Out[∘]=

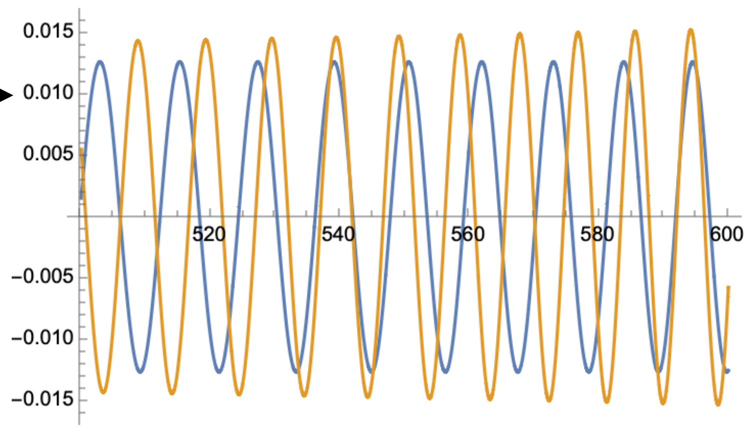


t = 1000, 400 < x < 500; overlay

```
In[∘]:= Plot[{Re[greenSNR[x, 1000]], Re[greenIMP0[x, 1000]]}, {x, 500, 600}, PlotRange → All, PlotPoints → 1000]
```

0.01

Out[∘]=

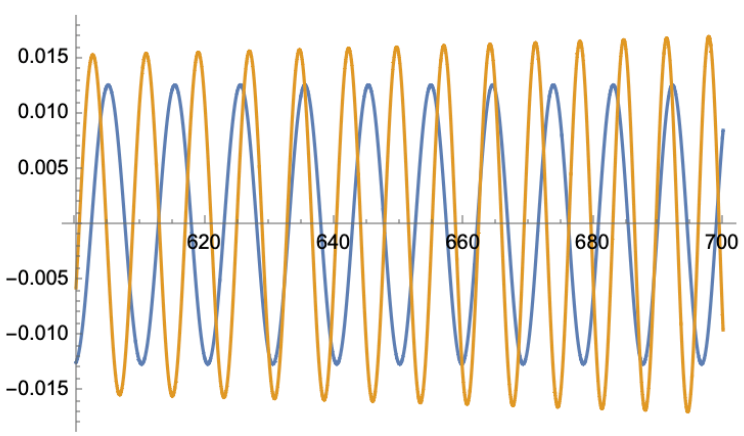


t = 1000, 500 < x < 600; overlay

```
In[∘]:= Plot[{Re[greenSNR[x, 1000]], Re[greenIMP0[x, 1000]]}, {x, 600, 700}, PlotRange → All, PlotPoints → 1000]
```

0.01

Out[∘]=

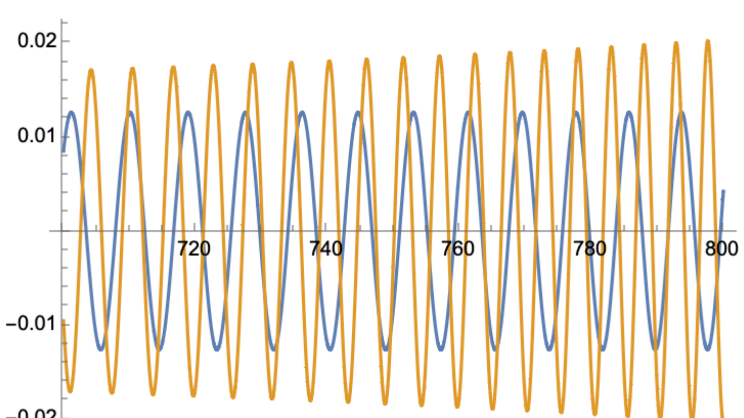


t = 1000, 600 < x < 700; overlay

```
In[∘]:= Plot[{Re[greenSNR[x, 1000]], Re[greenIMP0[x, 1000]]}, {x, 700, 800}, PlotRange → All, PlotPoints → 1000]
```

0.01

Out[∘]=

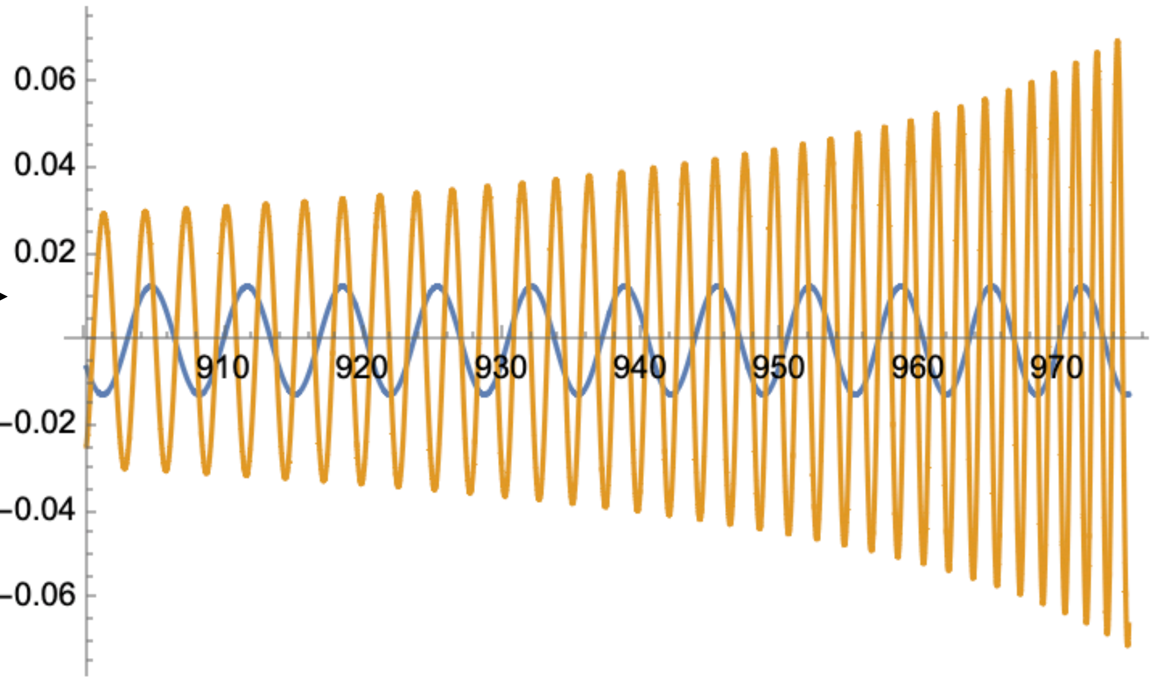


t = 1000, 700 < x < 800; overlay

```
In[∘]:= Plot[{Re[greenSNR[x, 1000]], Re[greenIMP0[x, 1000]]}, {x, 900, 975}, PlotRange → All, PlotPoints →
```

0.01 →

Out[∘]=

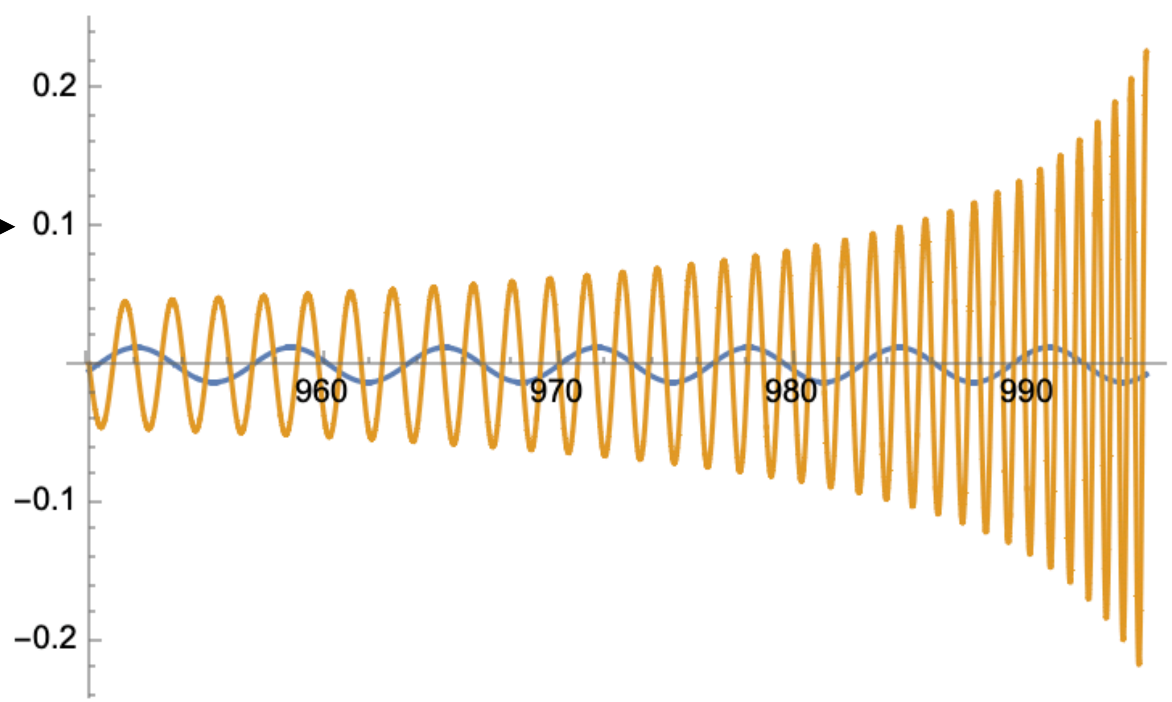


t = 1000, 900 < x < 975;
overlay

```
In[∘]:= Plot[{Re[greenSNR[x, 1000]], Re[greenIMP0[x, 1000]]}, {x, 950, 995}, PlotRange → All, PlotPoints →
```

0.1 →

Out[∘]=



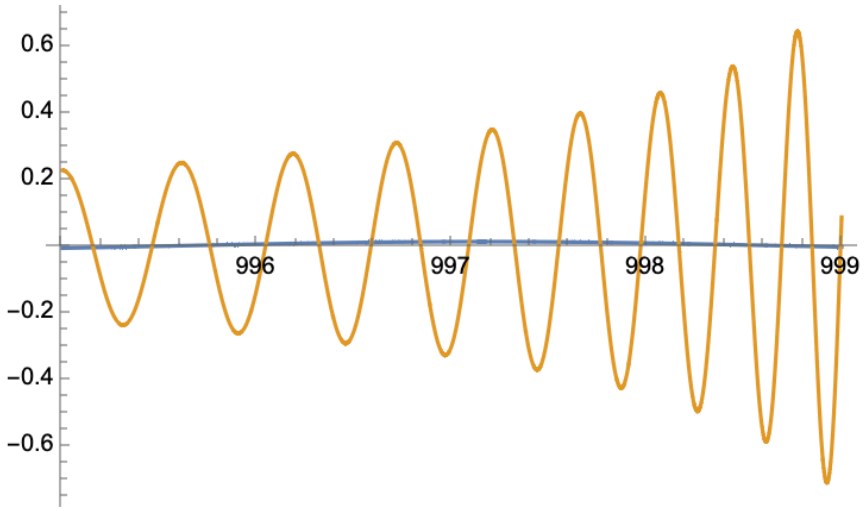
t = 1000, 950 < x < 995;
overlay

The improved Green function piles up at the light cone, before it suddenly dies:

```
In[•]:= Plot[{Re[greenSNR[x, 1000]], Re[greenIMP0[x, 1000]]}, {x, 995, 999}, PlotRange → All, PlotPoints → 1000]
```

0.4 →

Out[•]=

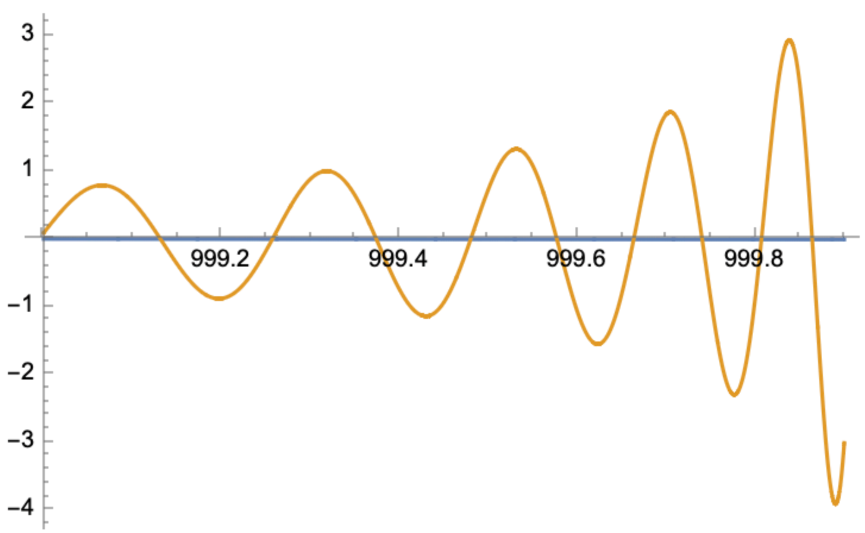


t = 1000, 995 < x < 999

```
In[•]:= Plot[{Re[greenSNR[x, 1000]], Re[greenIMP0[x, 1000]]}, {x, 999, 999.9}, PlotRange → All, PlotPoints → 1000]
```

2.0 →

Out[•]=

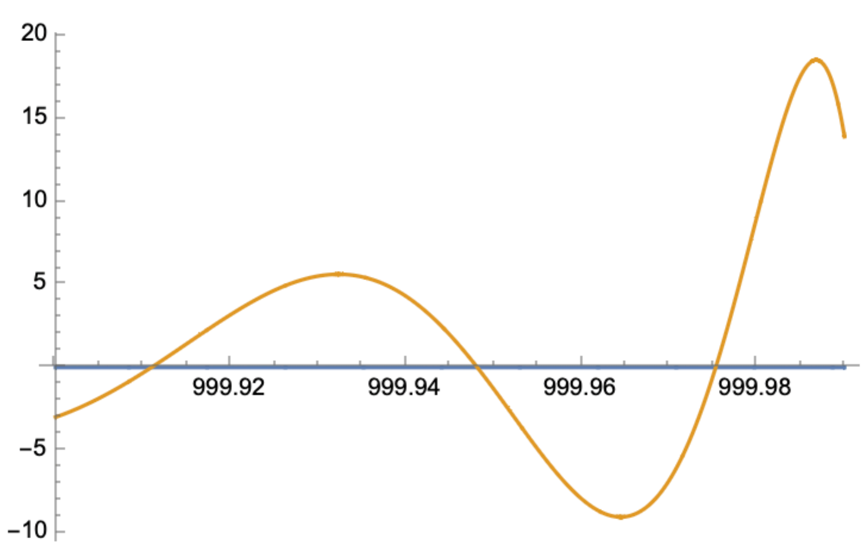


t = 1000, 999 < x < 999.9

```
In[•]:= Plot[{Re[greenSNR[x, 1000]], Re[greenIMP0[x, 1000]]}, {x, 999.9, 999.99}, PlotRange → All, PlotPoints → 1000]
```

15.0 →

Out[•]=

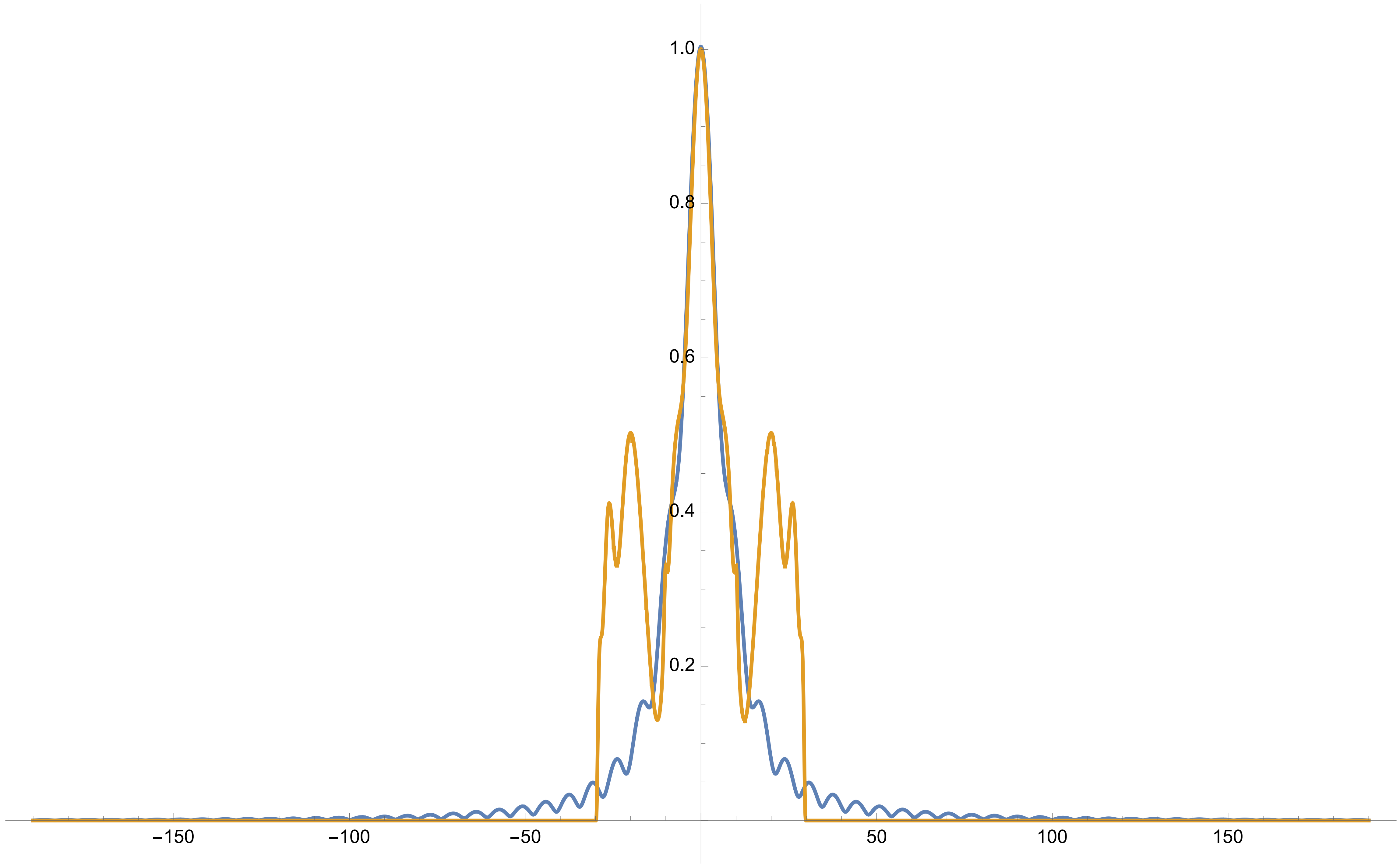


t = 1000, 999.9 < x < 999.99

This is bringing out a square root singularity approaching the light cone

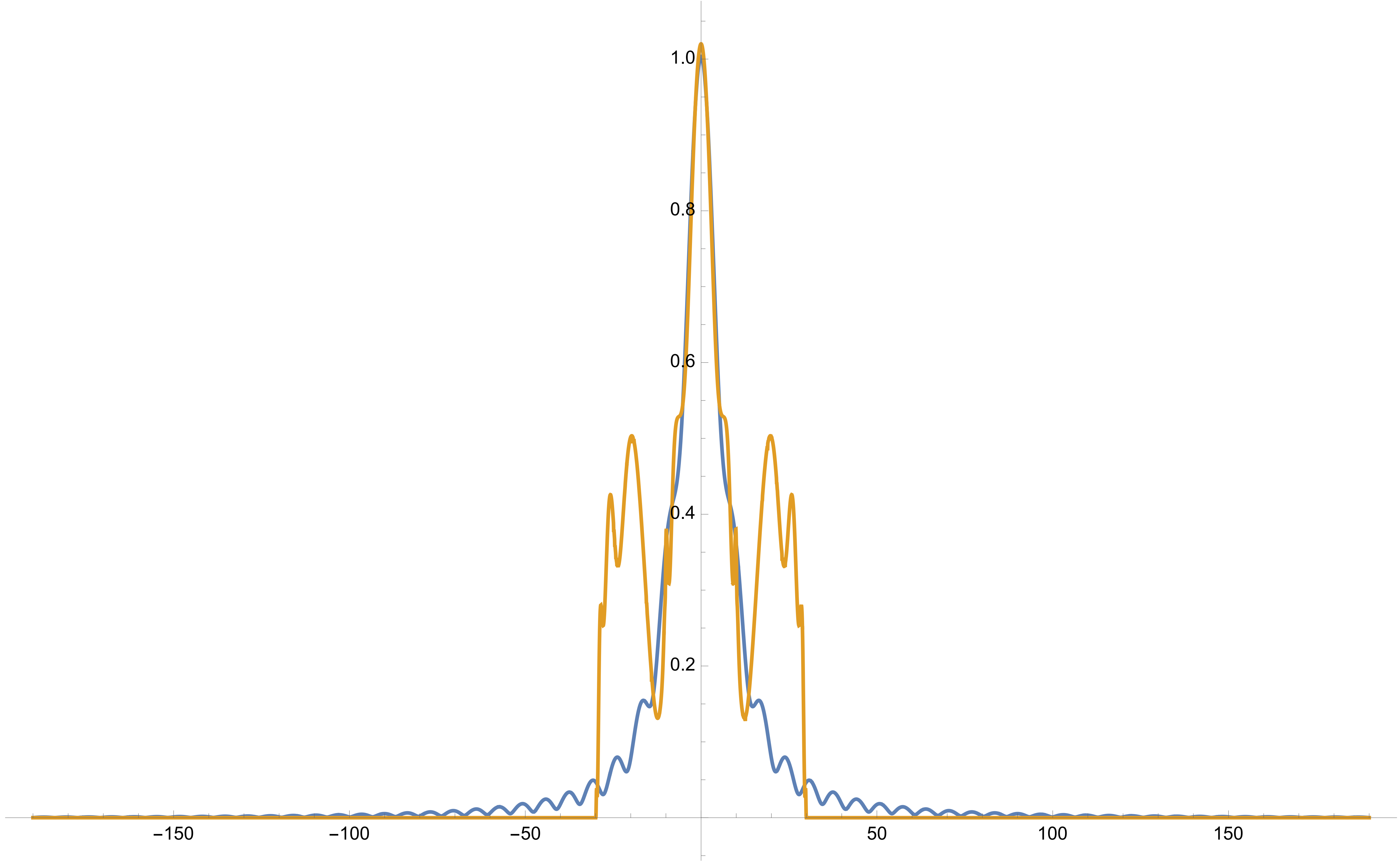
(3) Examples of Spreading

Speed Limit and Traffic Jam



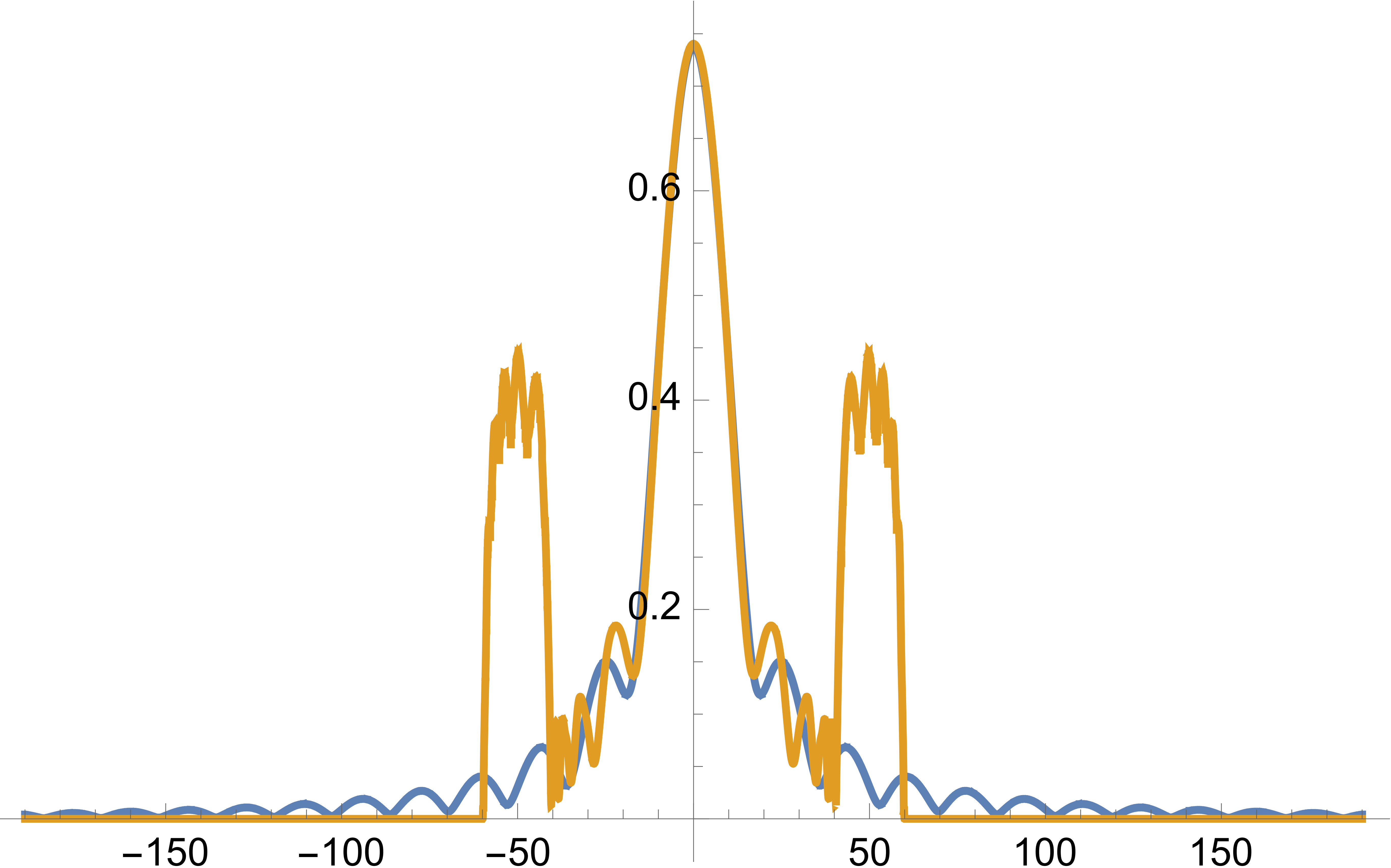
Smooth box with 2-sided width 20, evolved for 20 time steps.

Blue: NR Schrödinger; Gold: causal Schrödinger

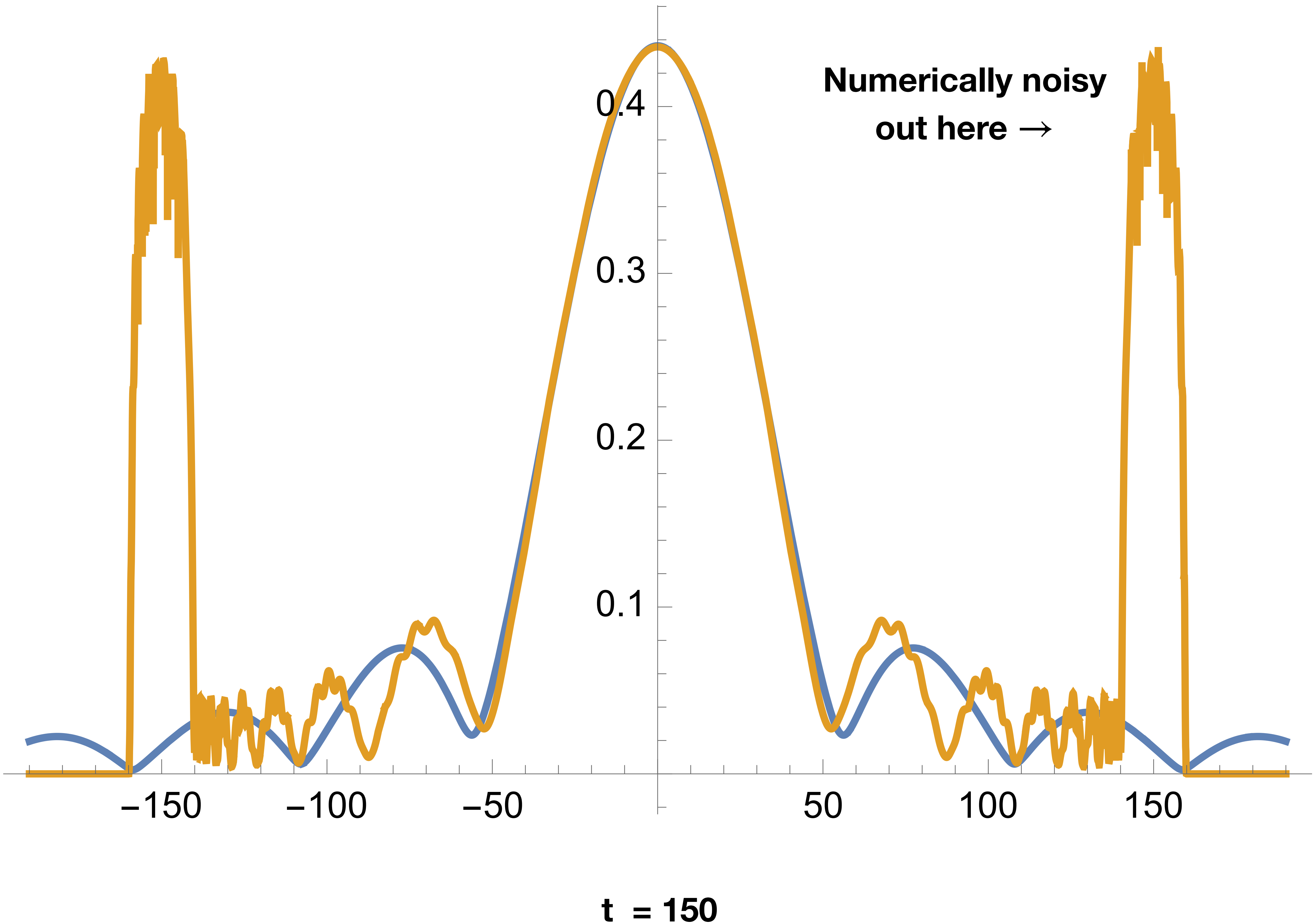


Smooth box with 2-sided width 20, evolved for 20 time steps.

Blue: NR Schrödinger; Gold: causal Schrödinger including improvement term



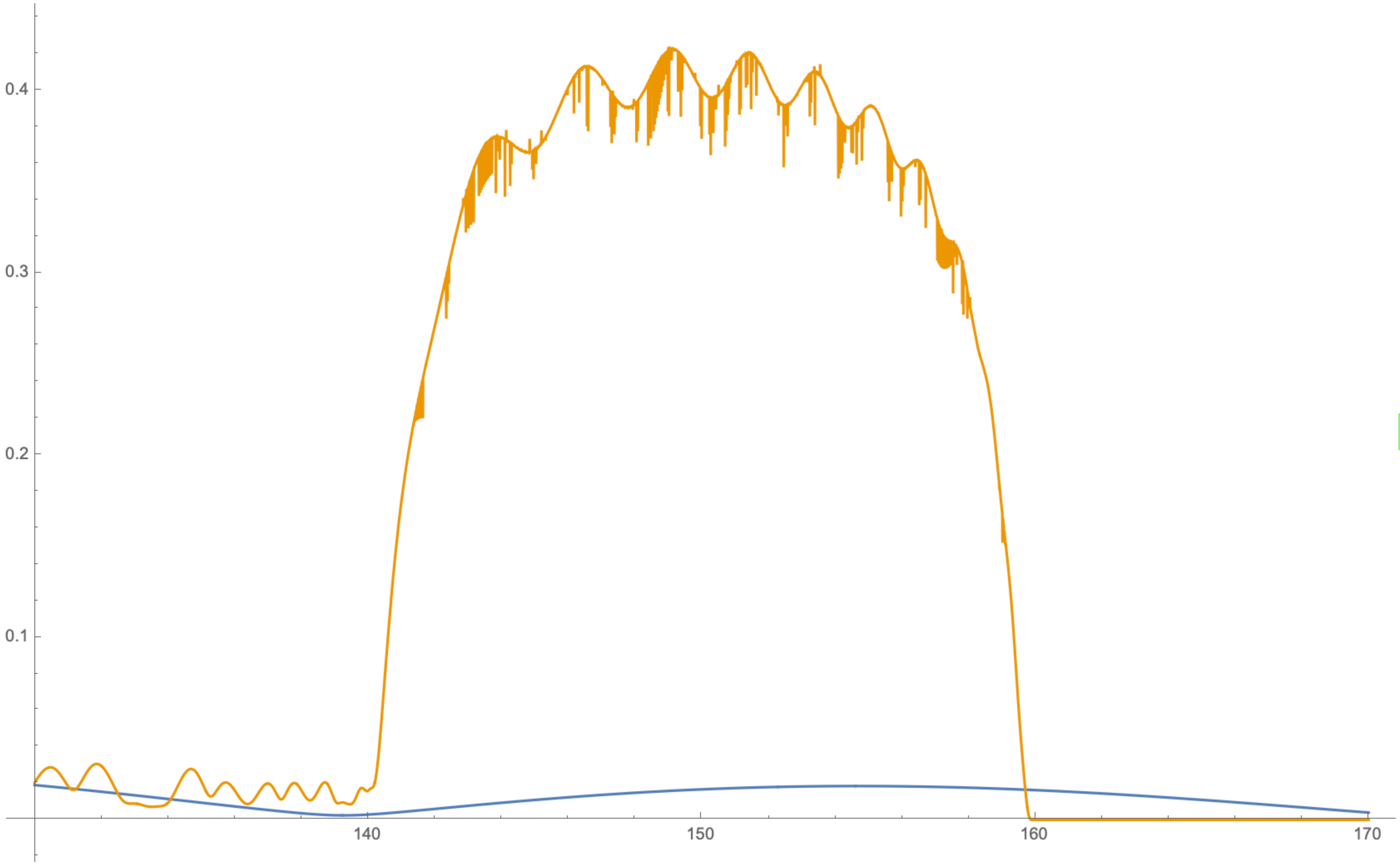
t = 50



Numerically noisy
out here →
0.4
0.3
0.2
0.1
−150
−100
−50
50
100
150
t = 150

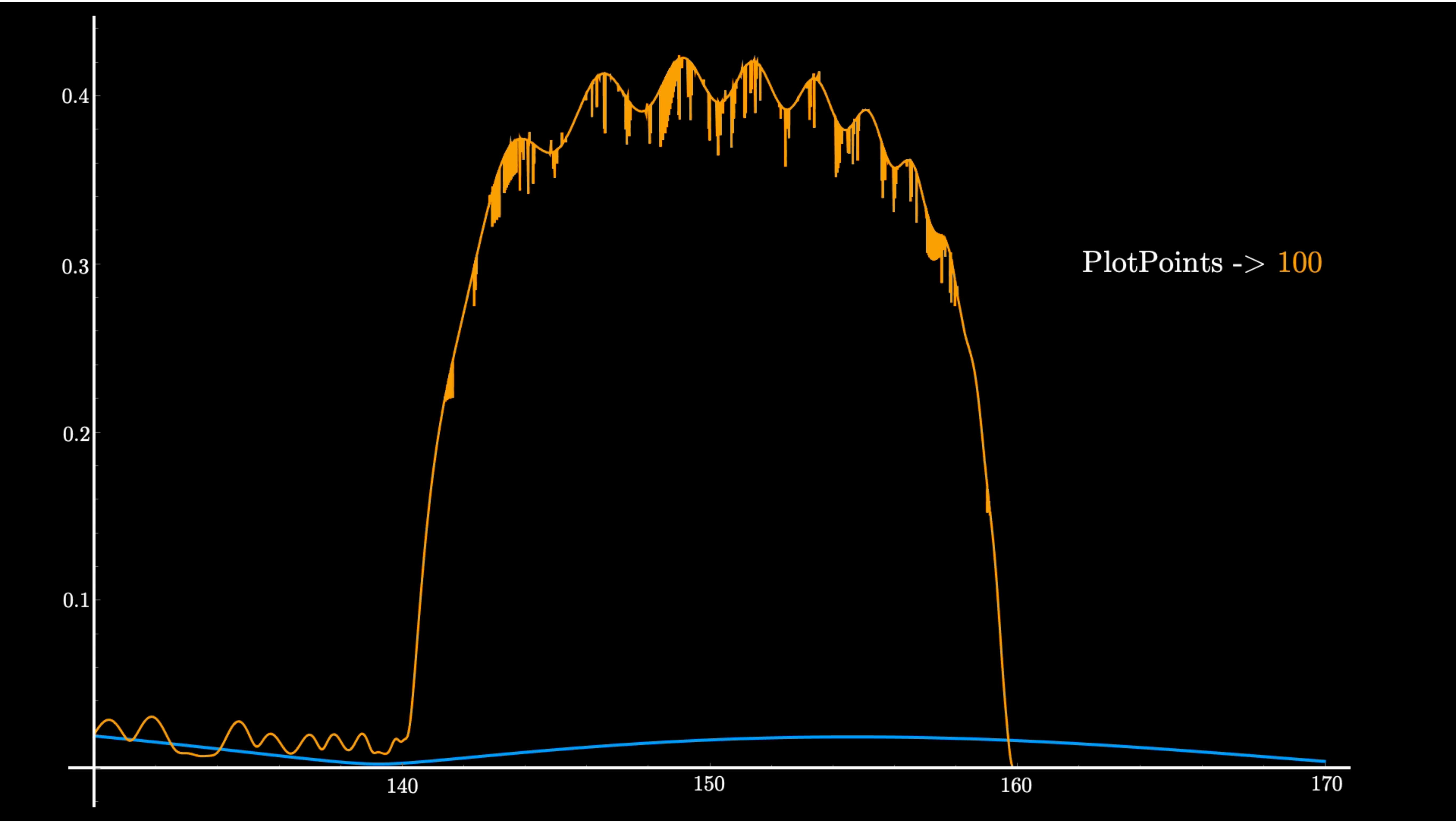
In[263]:= `Plot[{Abs[evolvedSmoothBoxSNR[10, x, 100]], Abs[evolvedSmoothBoxIMP1[10, x , 150]]}, {x, 130, 170}, PlotRange -> All, PlotPoints -> 100] // Timin`

Out[263]= {1609.05,



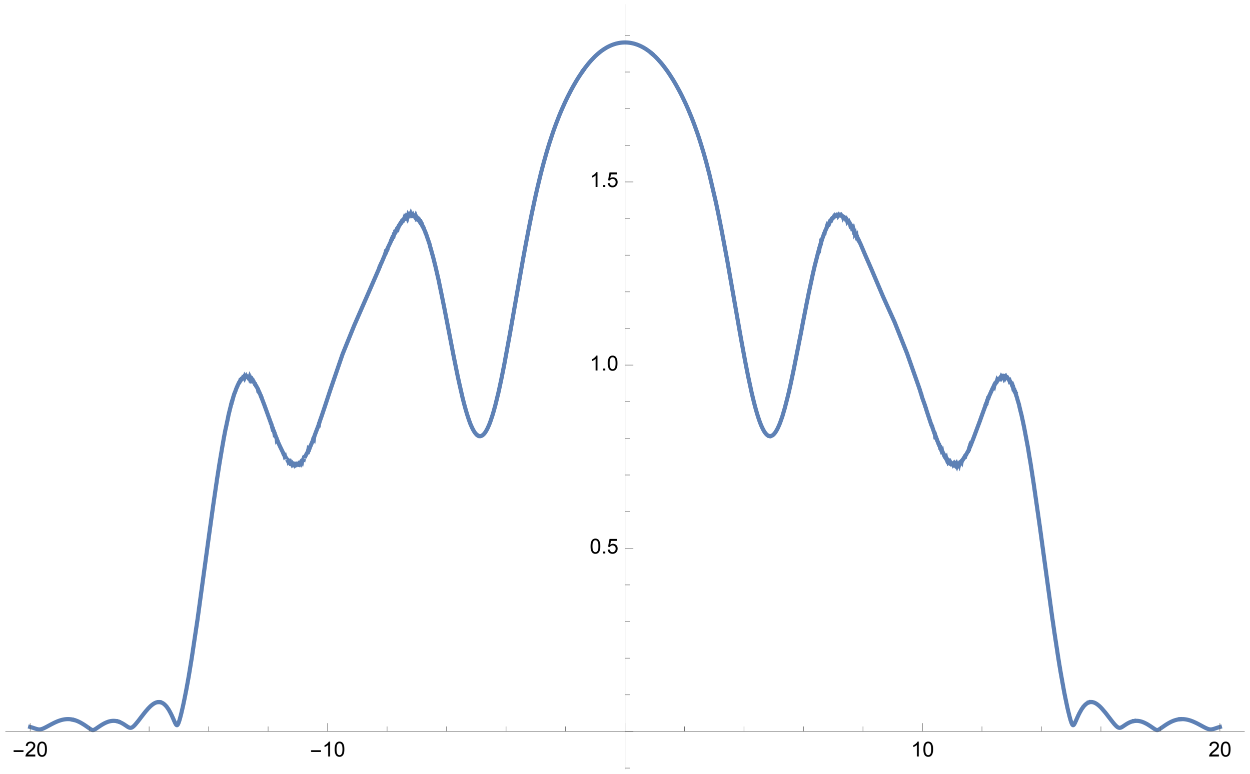
}

De-noised (imperfectly)

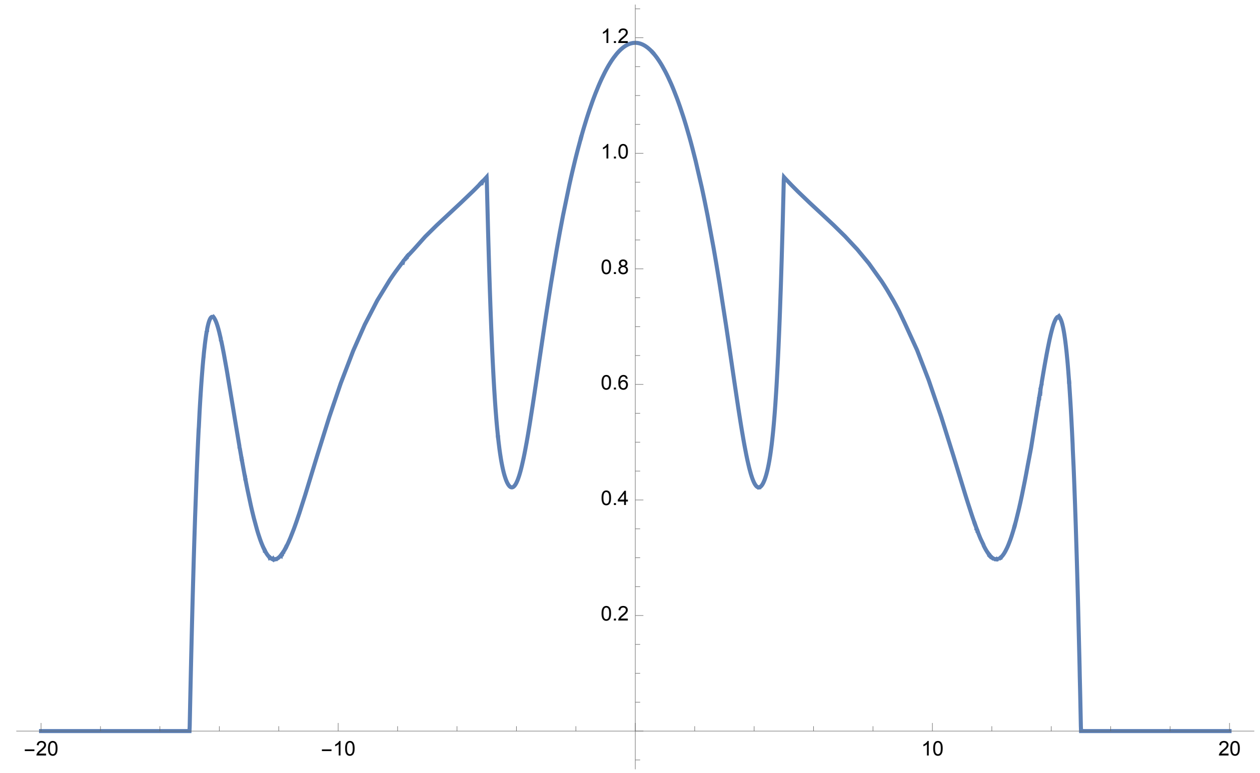


0.4
0.3
0.2
0.1
140
150
160
170
PlotPoints -> 100

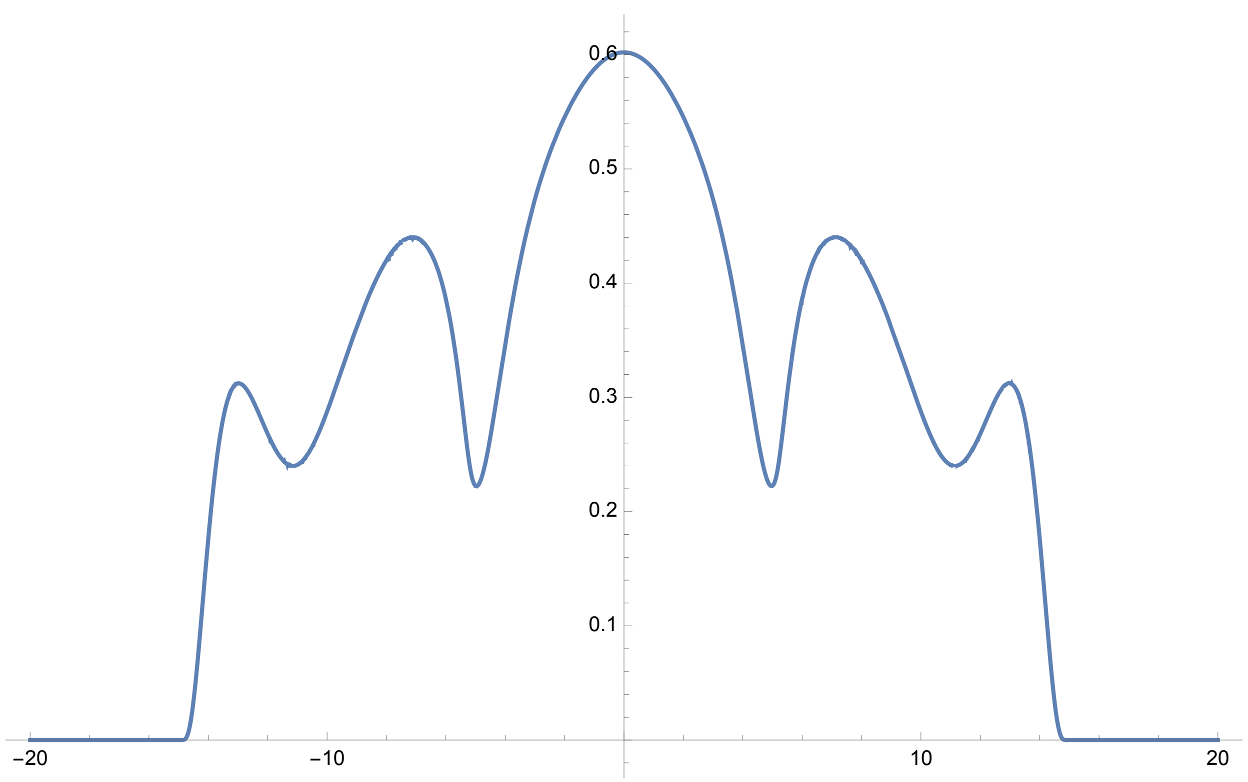
Important comment: The “traffic jam” does *not* appear to consist of high spatial frequency oscillations.



Filtered smooth box, width 10, time 10, low-pass filter k<=2

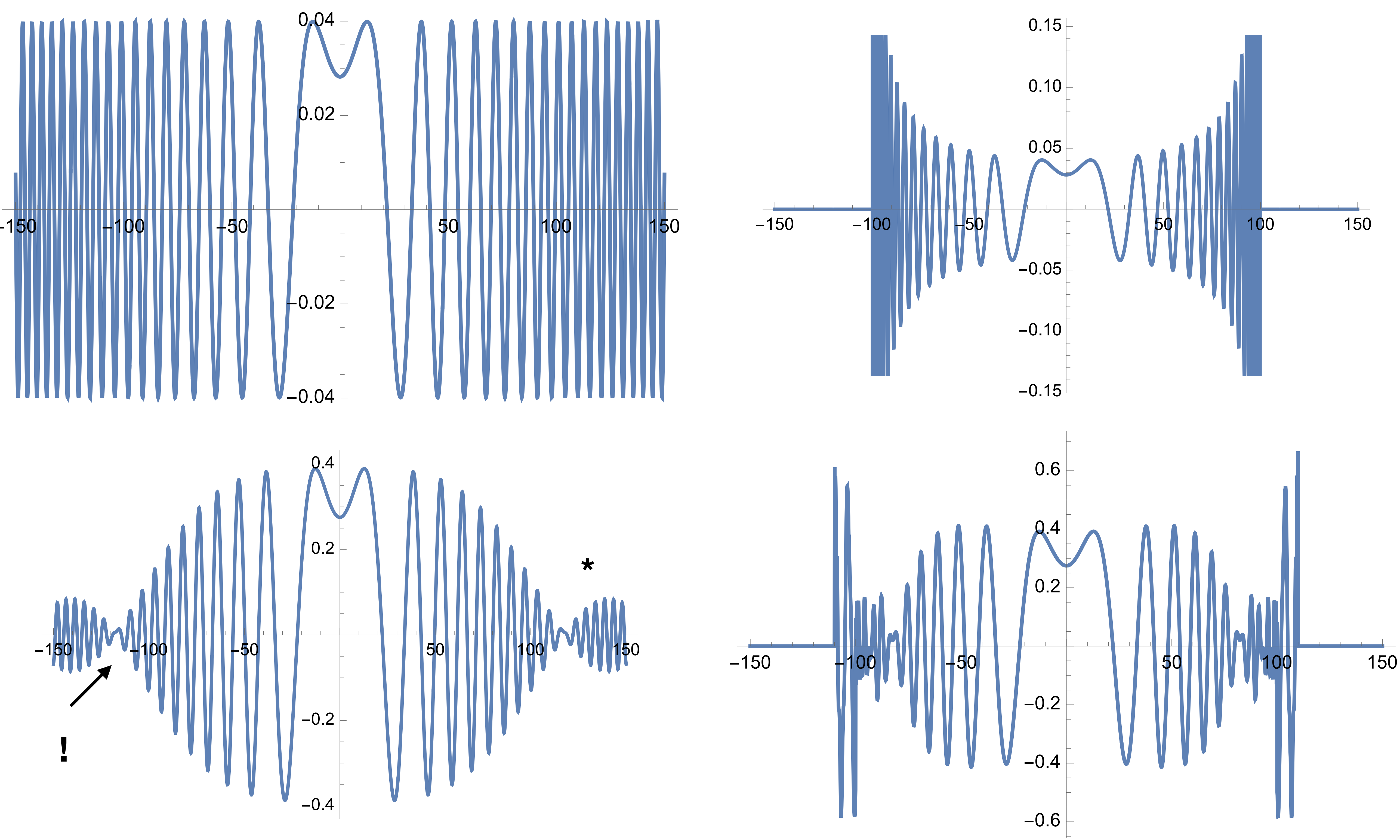


Box, width 10, time 10



Smooth box, width 10, time 10

The structure you observed depends upon your time resolution:

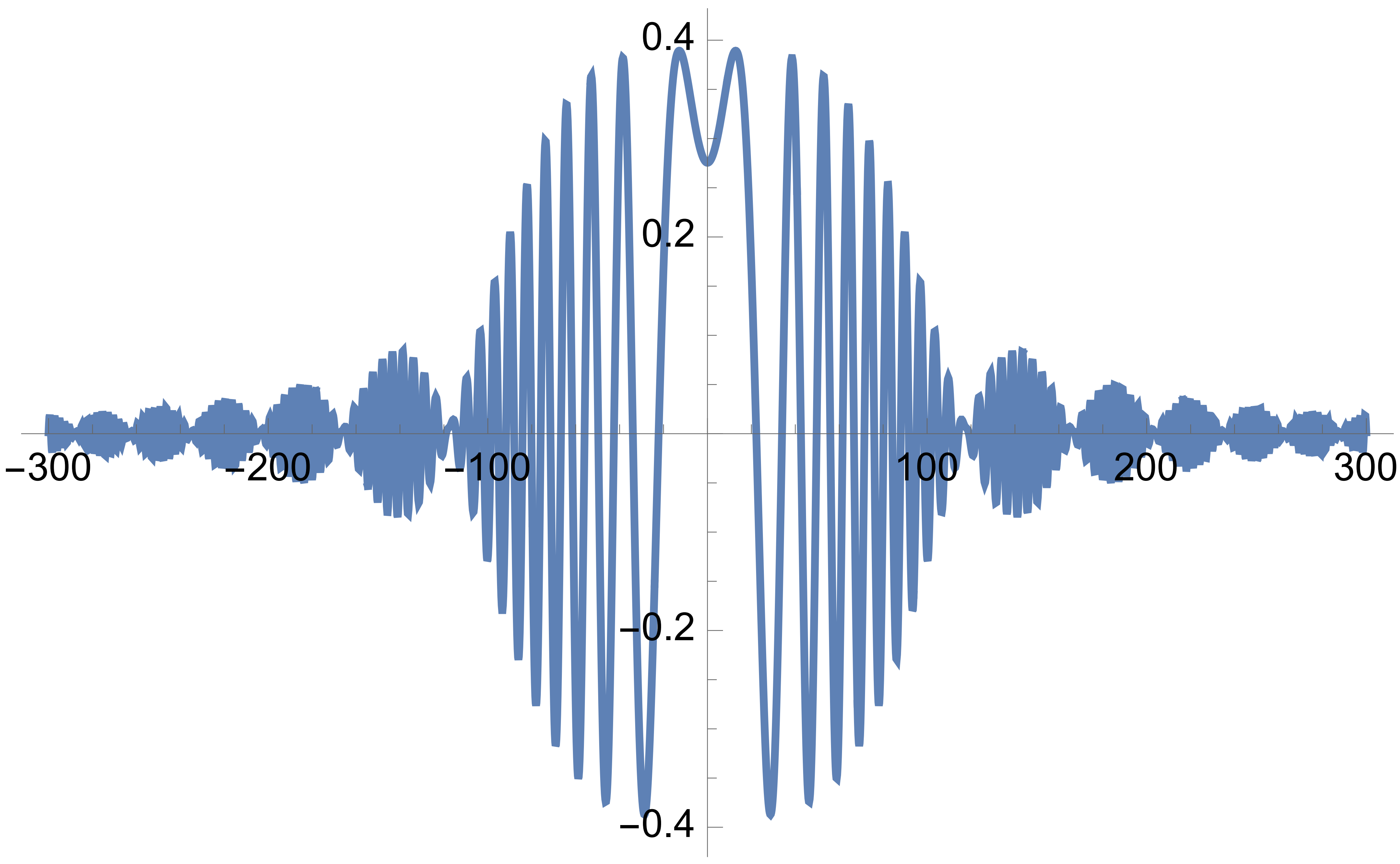


Real part of Green function at t = 100

Left: non-relativistic; Right: relativistic

Upper: Raw; Lower: smeared over 10 time steps

*


0.4
0.2
-0.2
-0.4
-300
-200
-100
100
200
300

(5) Interpretation as Selective Propagation

A Different $\sqrt{\mathbf{KG}}$

$$\partial_t^2 - \partial_x^2 + m^2 \;=\; (\partial_t + i\sqrt{m^2 - \partial_x^2})(\partial_t - i\sqrt{m^2 - \partial_x^2})$$

To propagate using the first factor (positive energy), we invert both and then multiply by the second:

$$G_{\text{pos.}} \;\sim\; (\partial_t - i\sqrt{m^2 - \partial_x^2})\, G^\tau$$

Now approximate to make it local, and take out the (trivial) rest mass factor:

$$G_{\text{cNR}}(x,t;x',0) \;=\; e^{imt}(\partial_t - im + \frac{i}{2m}\partial_x^2)\, G^\tau(x,t;x',0)$$

(5) Restoring Relativity, with Spin

Pauli to Dirac

To incorporate spin, we want to get causal propagation for a given 2-component wave function. (Also, Dirac is simply the right starting point for electrons.)

$$(i\gamma^\mu \partial_\mu - m)\,\phi \;=\; 0$$

$\Rightarrow$ Four functions instead of one. Fortunately, each of them satisfies KG.

We need to identify the NR limit and to identify where enough initial data comes from.

For the initial data:

$\phi = e^{-imt}\psi$ Expand in ∂_t / m *.

$$\begin{pmatrix} \partial_t & \sigma \cdot \nabla \\ -\sigma \cdot \nabla & -2im + \partial_t \end{pmatrix} \begin{pmatrix} \psi_B \\ \psi_S \end{pmatrix} = 0$$

$$\begin{aligned} \partial_t \psi_B + (\sigma \cdot \nabla)\psi_S &= 0 \\ \psi_S &= \frac{i\sigma \cdot \nabla}{2m}\psi_B \end{aligned}$$

These are enough to get $\psi_S(t=0)$ and $\partial_t \psi_B(t=0)$ from $\psi_B(t=0)$, and with $\partial_t \psi_S(t=0) = 0$ we're good to go.

Then we can propagate forward using the KG Green function technology.

Thus, component by component the behavior is covered by the same machinery as we have just discussed.

In this way, we will have solved

$$(i\gamma^\mu\partial_\mu - m)(i\gamma^\mu\partial_\mu + m)\,\psi_{\rm aux.} \;=\; 0\,.$$

We want to solve $(i\gamma^\mu\partial_\mu - m)\,\psi \;=\; 0$.

$\psi \;=\; (i\gamma^\mu\partial_\mu + m)\,\psi_{\rm aux.} \;=\; 0$ does the job!

Of course, this projection can be done once and for all at the level of Green functions.

We discussed how the NR limit works earlier, including interaction with external fields.

A noteworthy feature is that the corrected probability density

$\phi^*\phi \rightarrow \psi_B^*\psi_B + \dfrac{1}{4m^2}\,|\nabla\psi_B|^2$ at time 0, and

$\psi_B^*\psi_B + \psi_S^*\psi_S$ generally, is non-negative (unlike for KG) - indeed, generically it is *free of nodes!*

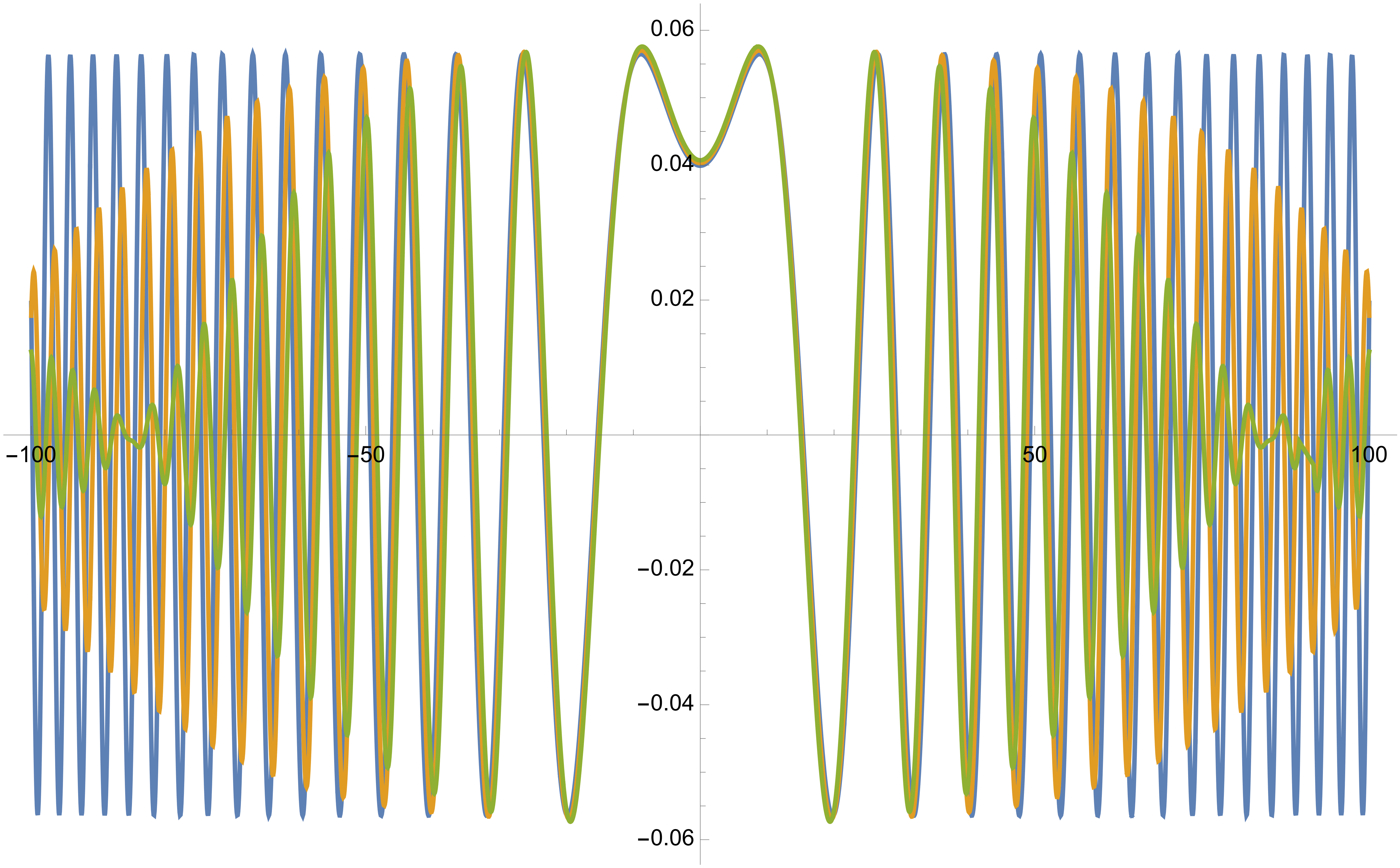
(6) Being Where You Shouldn't Be

Localizing in Space with Limited Energy
("Off Shell", "Under Barrier")


ABANDON ALL HOPE
YE WHO ENTER HERE

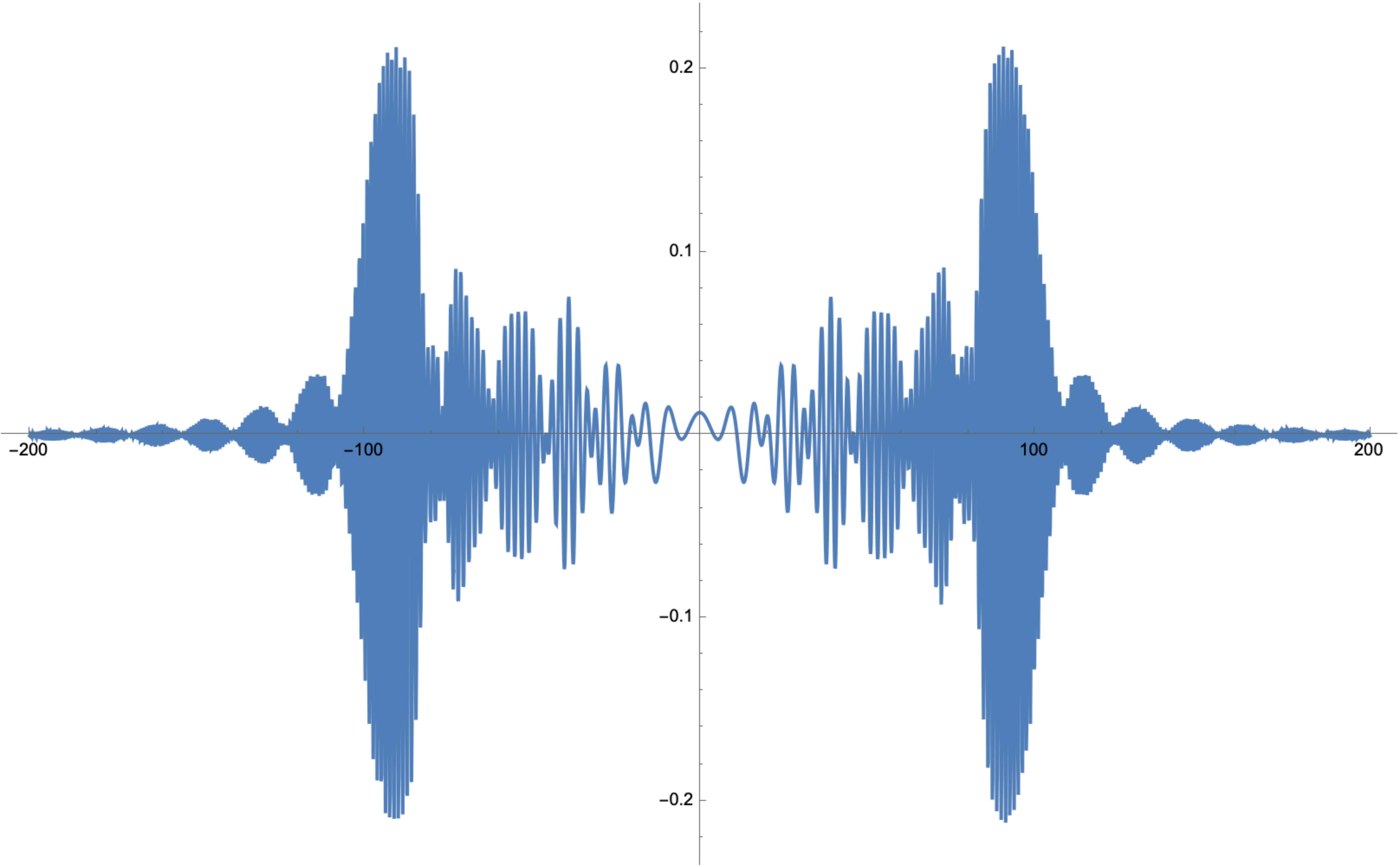
Using appropriate sources, we can put in lots of excitation “where it shouldn’t be”, or “off shell”.

Basically, one uses signal processing ideas (filtering) to generate small energy but large momentum fields in a confined space-time region, and see what happens.

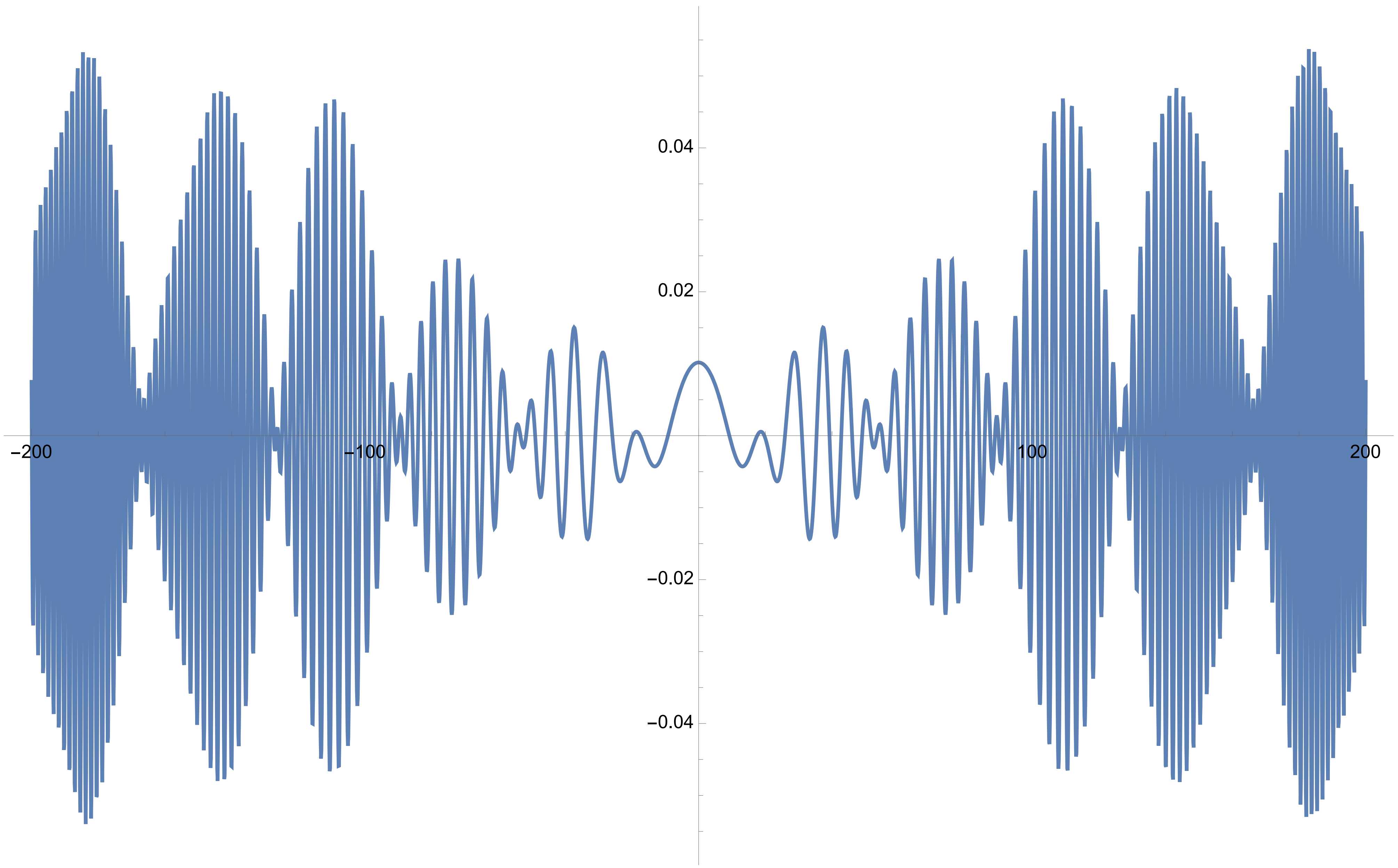


sourceTimeFilteredSNR[a_, x_, t_] :=
NIntegrate[greenSNR[x, t - s], {s, 0, a}, MinRecursion -> 8]

```
sourceTimeFilteredBoxCosSNR[tav_, yint_, k_, x_, t_] :=
NIntegrate[
greenSNR[x - y, t - s]*Cos[k*y]*Exp[I*k^2/s], {y, -yint,
yint}, {s, .01, tav} ]
```



Plot[Re[sourceTimeFilteredBoxCosSNR[4, 4, 5, x, 20]], {x, -200, 200}, PlotRange -> All] // Timing



t = 50