Journal Club
Institut für Theoretische Physik E, RWTH Aachen University
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Quantum-mechanical tunneling time of an electron wave packet

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I Tunneling delay time measurements in Helium

P. Eckle et al., Science 322 (2008) 1525

II Free wave packet

III Stationary solution for rectangular tunnel barrier

IV Numerical solution for time-dependent tunneling in three cases:

A: "Slow" wave packet, thin barrier → "tunneling of the low momenta"

B: "Slow" wave packet, thick barrier → "transmission of the high momenta"

C: "Fast" wave packet, thick barrier → time-resolved transmission

I Tunneling delay time measurements in Helium

P. Eckle[1], A.N. Pfeiffer[1], C. Cirelli[1], A. Staudte[2], R. Dörner[3], H.G. Muller[4], M. Büttiker[5], U. Keller[1], *Attosecond Ionization and Tunneling Delay Time Measurements in Helium*, **Science 322 (2008) 1525**

[1]ETH Zürich, [2]Ottawa, [3]Frankfurt, [4]Amsterdam, [5]Geneva

Aim: Measure the tunneling time of a bound electron through the Coulomb potential of a helium atom during ionization.

Measurement:

- Intense laser pulse hits helium atoms → lowers Coulomb potential → enables tunneling of bound electron to the outside → ionization
- At the exit of the tunnel the electron is accelerated by electric laser field → laser polarization determines direction of electron drift momentum
- Use circularly/elliptically polarized laser pulse → electron drift direction corresponds to laser field polarization at the time of tunnel exit → time measurement with attosecond accuracy ("angular streaking")
- Measure drift of helium instead of electrons → correspondence by simple semi-classical simulation assuming instantaneous tunneling (with Coulomb correction)

Calibration of absolute time zero:

- ellipticity of laser polarization induces oscillations in the angular ion momentum distributions
- calibration by linear polarized laser pulse

Result: upper limit of 34 as for tunneling time
(intensity-averaged upper limit: 12 as)

Comparison to theoretical predictions:

- Instantaneous tunneling agrees with numerical simulations
- Wigner–Eisenbud–Smith delay time: follow peak of a wave packet;
  delay time can be much shorter than time for light propagation ("superluminal")
- Buttiker-Landauer traversal time: modulating tunnel barrier height in time;
  predicts 450–560 as for present conditions

II Free wave packet

Schrödinger equation in 1 dimension ($\hbar = 1$): $i\partial_t \psi(t,x) = \left(-\frac{\partial_x^2}{2m} + V(x)\right)\psi(t,x)$

Free electron wave (without barrier potential, $V \equiv 0$):

single-momentum contribution (Fourier component): $\tilde{\psi}_{\text{free}}(k;t,x) = \exp\left(ikx - i\frac{k^2}{2m}t\right)$

Gaussian wave packet: amplitude $A(k) = \frac{1}{\sqrt[4]{2\pi}}\frac{1}{\sqrt{\sigma_k}}\exp\left(-\frac{(k-k_0)^2}{4\sigma_k^2} - ikx_0\right)$

$\hookrightarrow$ normalized momentum distribution $|A(k)|^2 = \frac{1}{\sqrt{2\pi}}\frac{1}{\sigma_k}\exp\left(-\frac{(k-k_0)^2}{2\sigma_k^2}\right)$

with $\langle k\rangle = \int_{-\infty}^{\infty} \mathrm{d}k\, k\, |A(k)|^2 = k_0$ and $\sigma_k = \sqrt{\langle k^2\rangle - \langle k\rangle^2}$

Time-dependent free wave packet: integration of $\tilde{\psi}_{\text{free}}$ over k with amplitudes A

$$\psi_{\text{free}}(t,x) = \int_{-\infty}^{\infty} \frac{\mathrm{d}k}{\sqrt{2\pi}}\, A(k)\, \tilde{\psi}_{\text{free}}(k;t,x)$$

$\hookrightarrow$ Fourier transformation with factor e^{ikx} included in $\tilde{\psi}_{\text{free}}(k;t,x)$

Time-dependent free wave packet: analytical solution

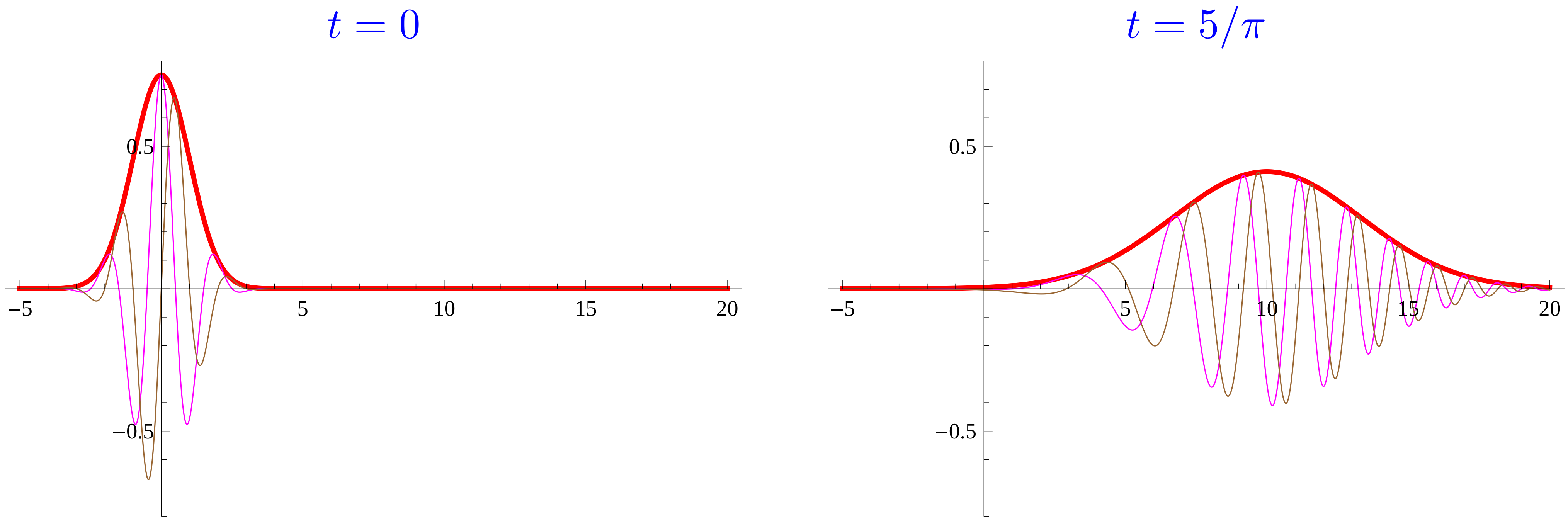
$$\psi_{\text{free}}(t,x) = \frac{1}{\sqrt[4]{2\pi}} \sqrt{\frac{2\sigma_k}{1 + i\frac{2\sigma_k^2}{m}t}} \exp\left(\frac{-\sigma_k^2 (x-x_0)^2 + i k_0 (x-x_0) - i\frac{k_0^2}{2m}t}{1 + i\frac{2\sigma_k^2}{m}t} \right)$$

$\hookrightarrow$ normalized probability distribution

$$|\psi_{\text{free}}(t,x)|^2 = \frac{1}{\sqrt{2\pi}} \frac{2\sigma_k}{\sqrt{1 + \frac{4\sigma_k^4}{m^2}t^2}} \exp\left(-\frac{1}{2} \frac{(2\sigma_k)^2}{1 + \frac{4\sigma_k^4}{m^2}t^2} \left[x - \left(x_0 + \frac{k_0}{m}t \right) \right]^2 \right)$$

with $\langle x \rangle = \int_{-\infty}^{\infty} \mathrm{d}x\, x\, |\psi_{\text{free}}(t,x)|^2 = x_0 + \frac{k_0}{m}t$ and $\sigma_x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \frac{\sqrt{1 + \frac{4\sigma_k^4}{m^2}t^2}}{2\sigma_k}$

Free wave packet with parameters $k_0 = \pi$, $\sigma_k = 1/\sqrt{2} \approx 0.7$, $x_0 = 0$, $2m = 1$,
plot $|\psi_{\text{free}}(t,x)|$, $\text{Re}\,\psi_{\text{free}}(t,x)$ and $\text{Im}\,\psi_{\text{free}}(t,x)$:



Velocity of the packet maximum: $v = \dfrac{k_0}{m} = 2k_0 = 2\pi$,
but the front of the wave packet is faster!

Numerical integration of Fourier components $A(k)\,\tilde{\psi}_{\text{free}}(k;t,x) \Rightarrow$ same result.

III Stationary solution for rectangular tunnel barrier

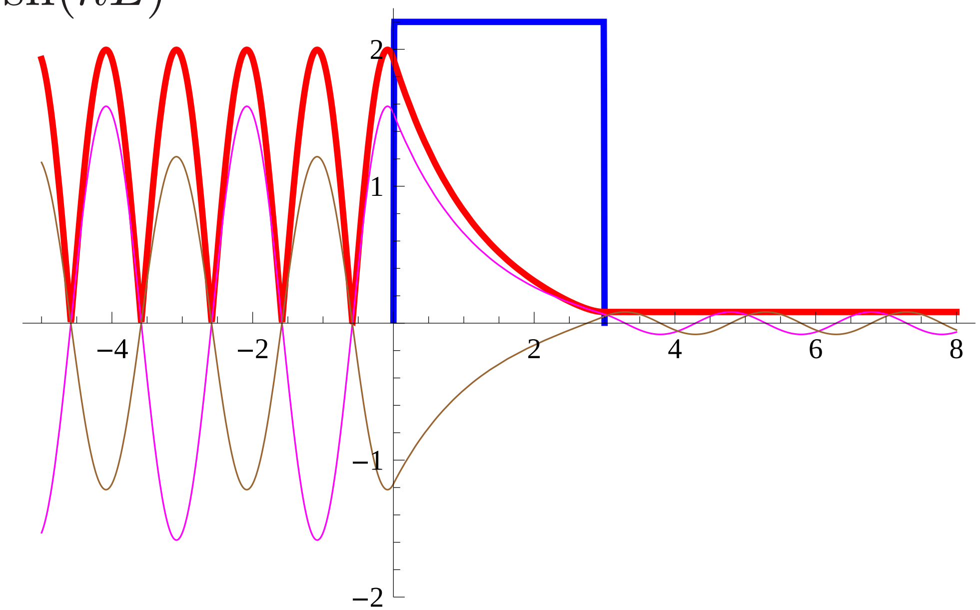
Rectangular tunnel barrier with height V and length L: $V(x) = V\,\theta(x)\theta(L-x)$

Stationary solution for incoming momentum k:

$$\tilde{\psi}(k;t,x) = \exp\left(-i\frac{k^2}{2m}t\right)\begin{cases} e^{ikx} + \frac{(k^2+\kappa^2)\sinh(\kappa L)}{\Delta(k,\kappa)}\,e^{-ikx}\,, & x \le 0, \\ \frac{k(k+i\kappa)}{\Delta(k,\kappa)}\,e^{-\kappa(x-L)} - \frac{k(k-i\kappa)}{\Delta(k,\kappa)}\,e^{\kappa(x-L)}\,, & 0 \le x \le L, \\ \frac{2ik\kappa}{\Delta(k,\kappa)}\,e^{ik(x-L)}\,, & L \le x \end{cases}$$

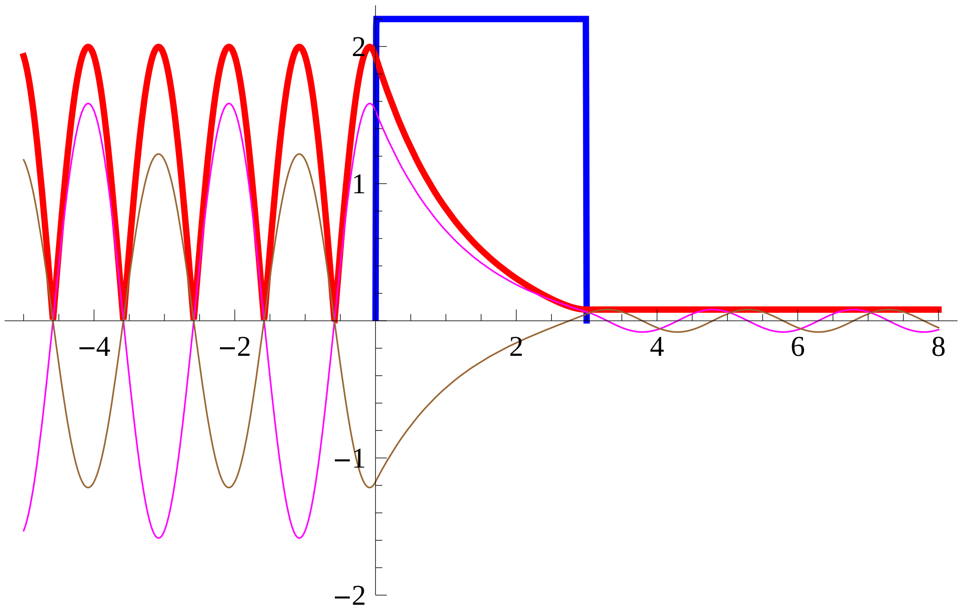
with $\Delta(k,\kappa) = (k^2-\kappa^2)\sinh(\kappa L) + 2ik\kappa\cosh(\kappa L)$
and $\kappa = \sqrt{2mV - k^2}$
(or $\kappa = -i\sqrt{k^2 - 2mV}$ for $k^2 > 2mV$)

Example for $k^2 < 2mV$:
plot barrier (height in arbitrary units),
$|\tilde{\psi}(k;t,x)|$, $\mathrm{Re}\,\tilde{\psi}(k;t,x)$ and $\mathrm{Im}\,\tilde{\psi}(k;t,x)$

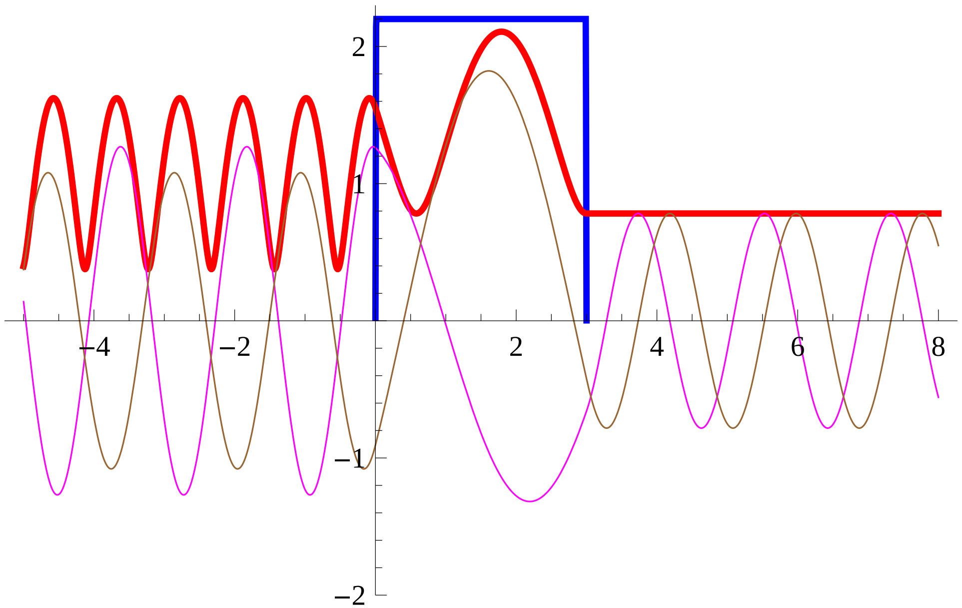


Stationary solution for $L = 3$ and $\sqrt{2mV} = 3.25$:

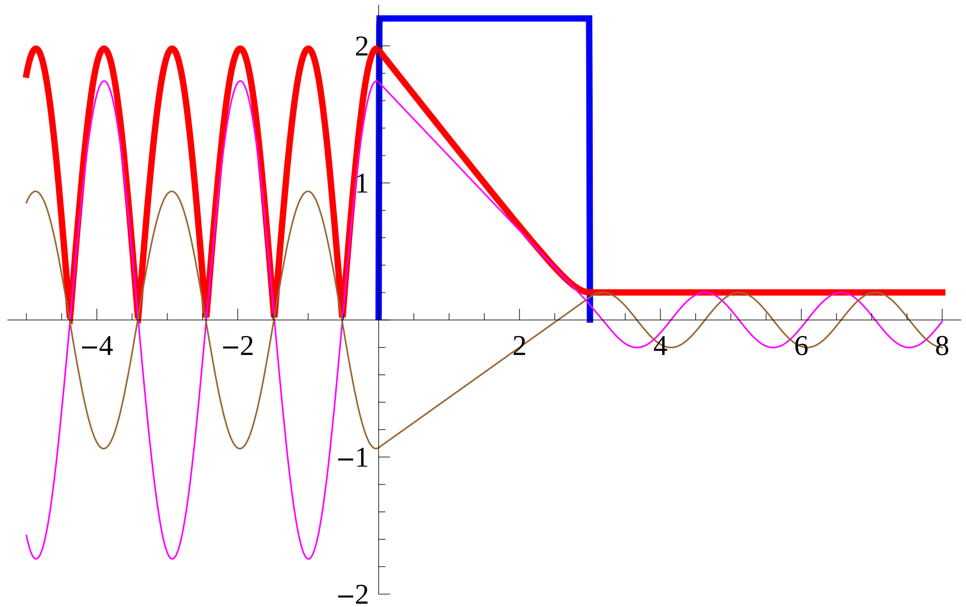
$k = \pi < \sqrt{2mV}$



$k = 3.5 > \sqrt{2mV}$



$k = \sqrt{2mV}$



IV Numerical solution for time-dependent tunneling

Multiply stationary solution $\tilde{\psi}(k;t,x)$ with Gaussian wave packet $A(k)$ and integrate numerically over k:

$$\psi(t,x) = \int_{-\infty}^{\infty} \frac{\mathrm{d}k}{\sqrt{2\pi}} A(k)\,\tilde{\psi}(k;t,x)$$

Numerical integration performed by MATHEMATICA with a working precision of 20–35 digits, depending on the parameters.

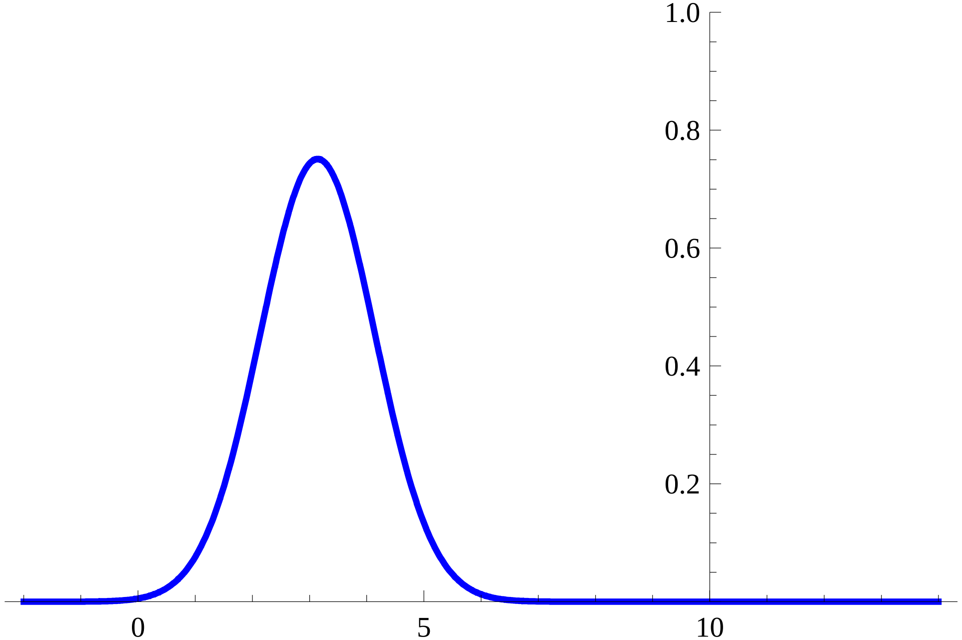
Three cases:

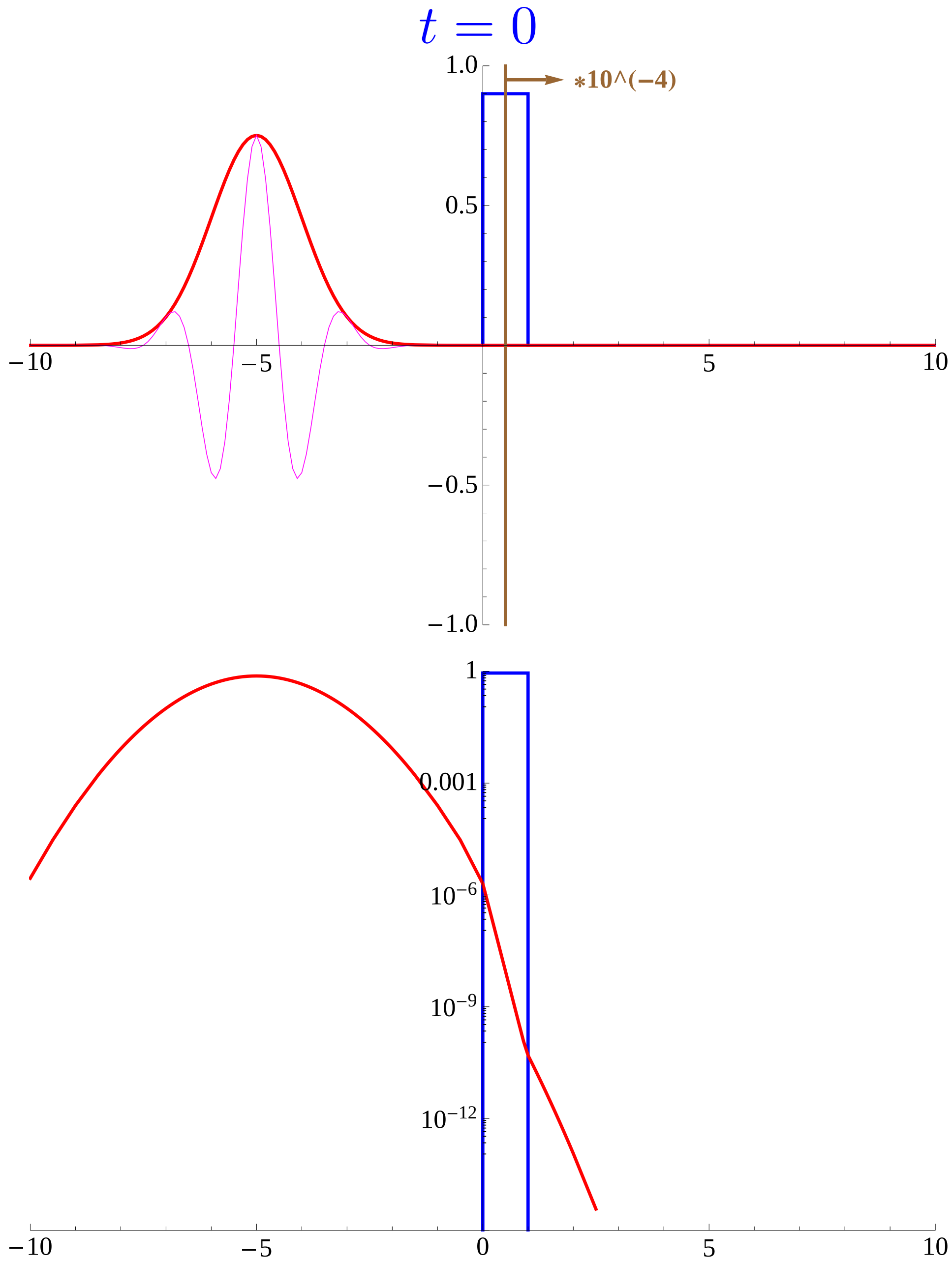
A: "slow" wave packet ($k_0 = \pi \gtrsim \sigma_k$), thin barrier ($L = 1 = \pi/k_0 \sim \sigma_x$)
B: "slow" wave packet ($k_0 = \pi \gtrsim \sigma_k$), thick barrier ($L = 5 > \{\sigma_x, \pi/k_0\}$)
C: "fast" wave packet ($k_0 = 20 \gg \sigma_k$), thick barrier ($L = 5 > \sigma_x \gg \pi/k_0$)

A: “Slow” wave packet, thin barrier

Parameters: $k_0 = \pi \gtrsim \sigma_k$,
$L = 1 = \pi/k_0 \sim \sigma_x$, $\sigma_k = 1/\sqrt{2} \approx 0.7$,
$x_0 = -5$, $2m = 1$, $V = 10^2 \gg k_0^2$

Momentum distribution $|A(k)|$:

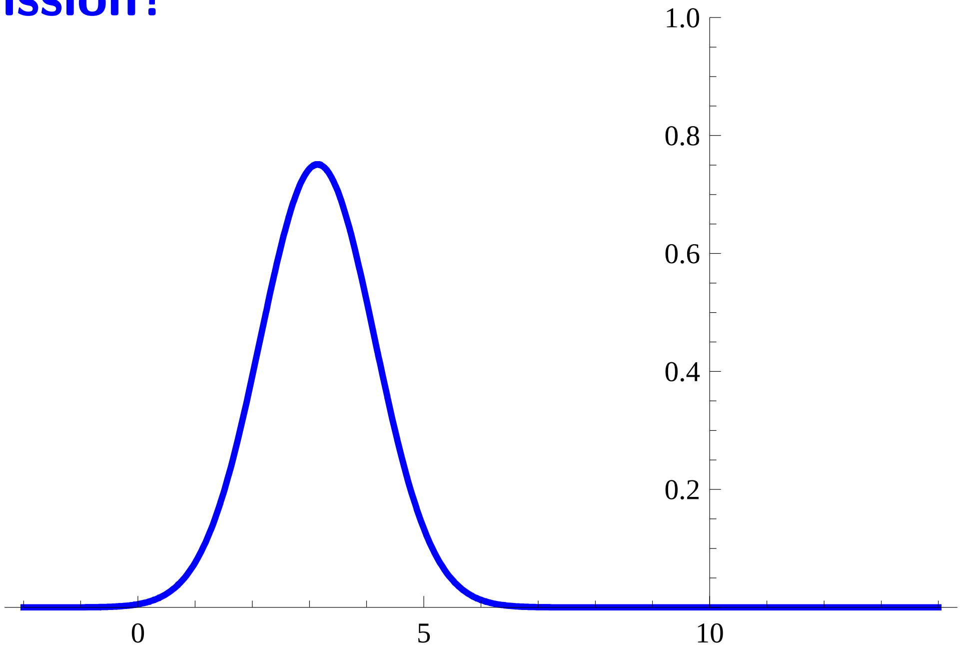




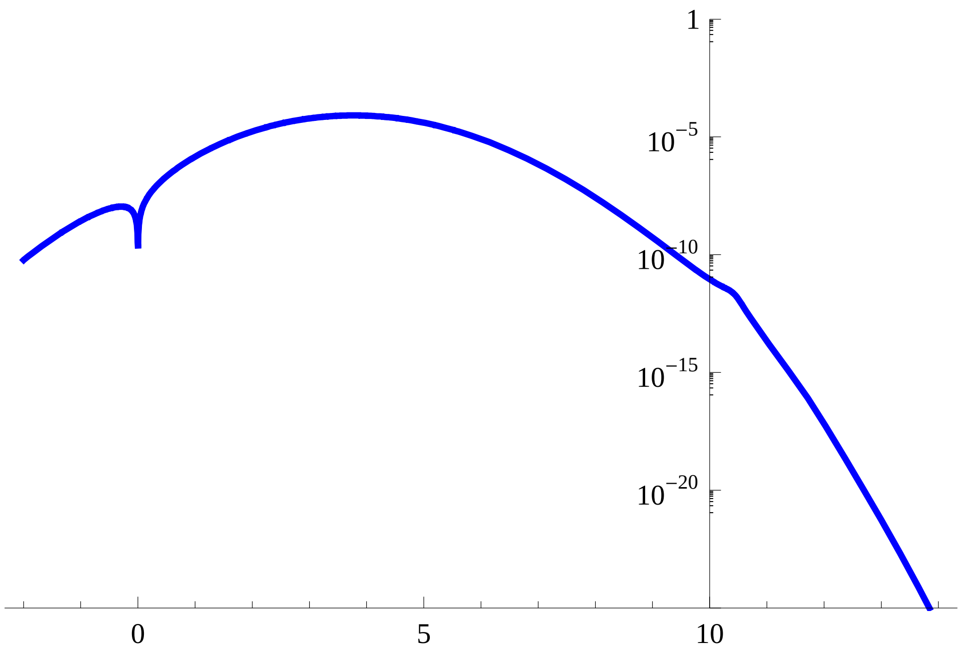
Right plots: barrier, $|\psi(t,x)|$, $\mathrm{Re}\,\psi(t,x)$;
top: to scale by 10^{-4} for $x > 0.5$;
bottom: logarithmic scale

A: "Slow" wave packet, thin barrier — Which momenta contribute to the transmission?

Momentum distribution of incoming wave packet, i.e. part of $\tilde{\psi}(k;t,x) \propto e^{ikx}$ at $x < 0$: $|A(k)|$



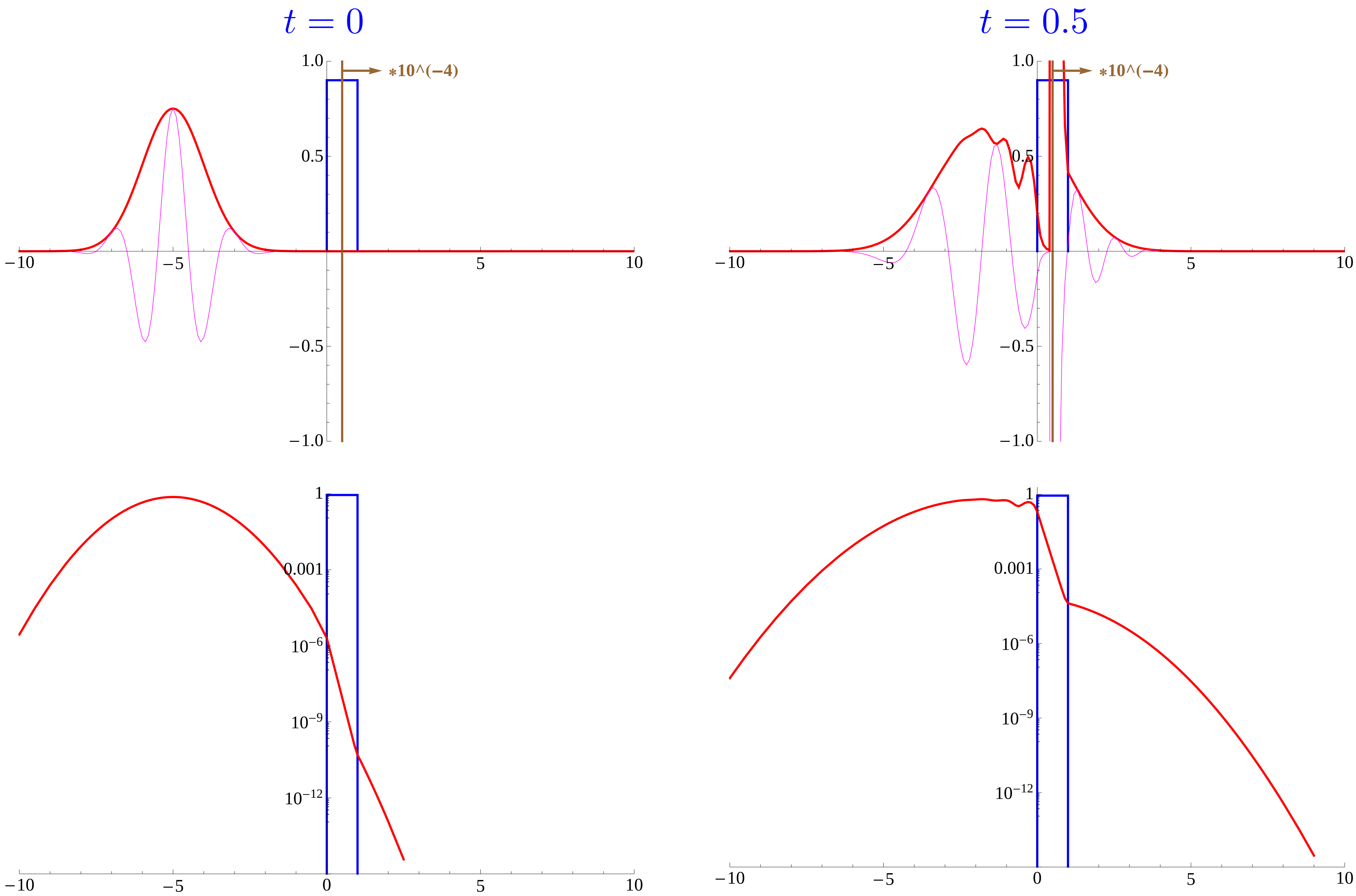
Momentum distribution of transmitted wave packet, i.e. $\tilde{\psi}(k;t,x)$ at $x > L$: $|A(k)\,\tilde{\psi}(k;t,L)|$ (logarithmic scale)



⇒ transmission dominated by central momenta $k \approx k_0 < \sqrt{V}$

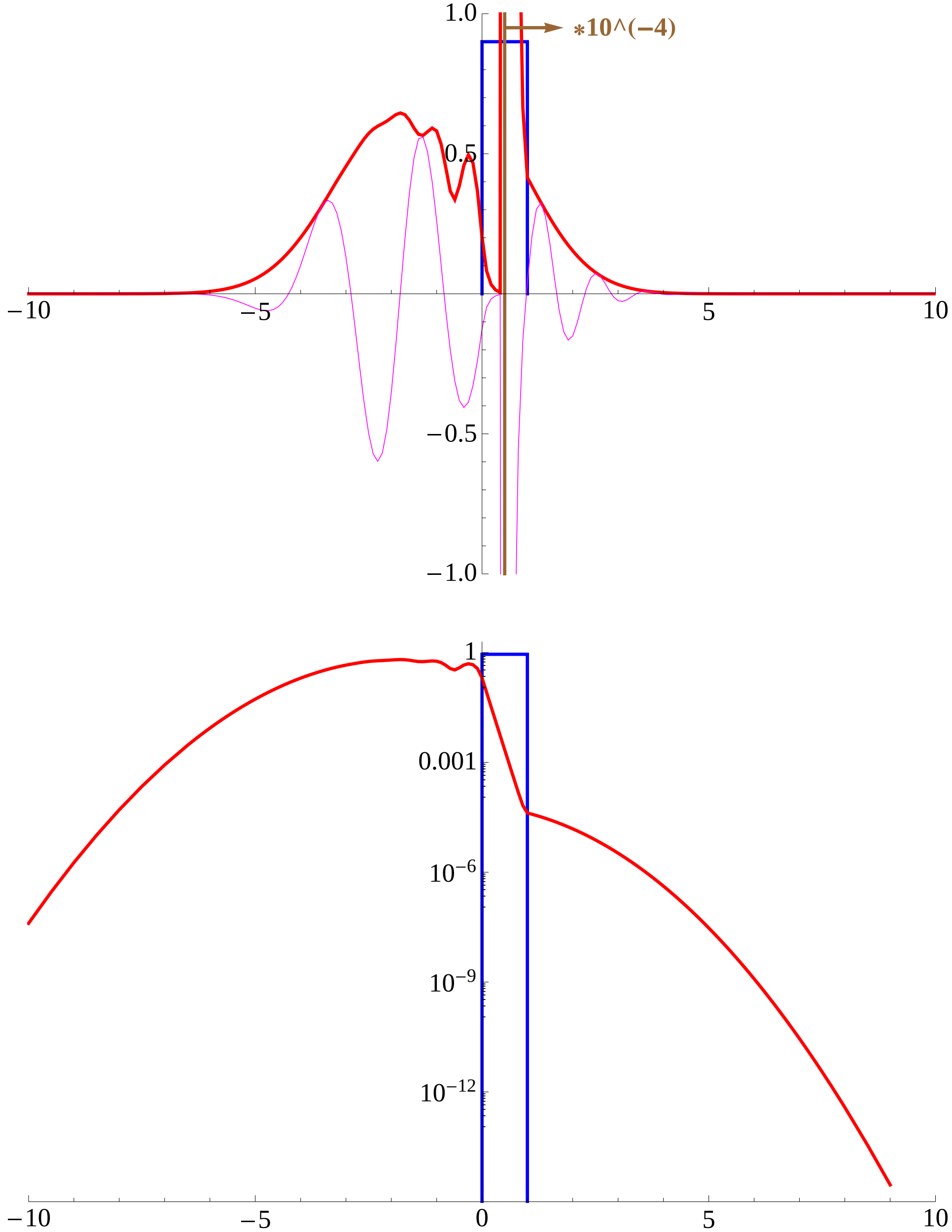
⇒ "real" tunneling

A: "Slow" wave packet, thin barrier

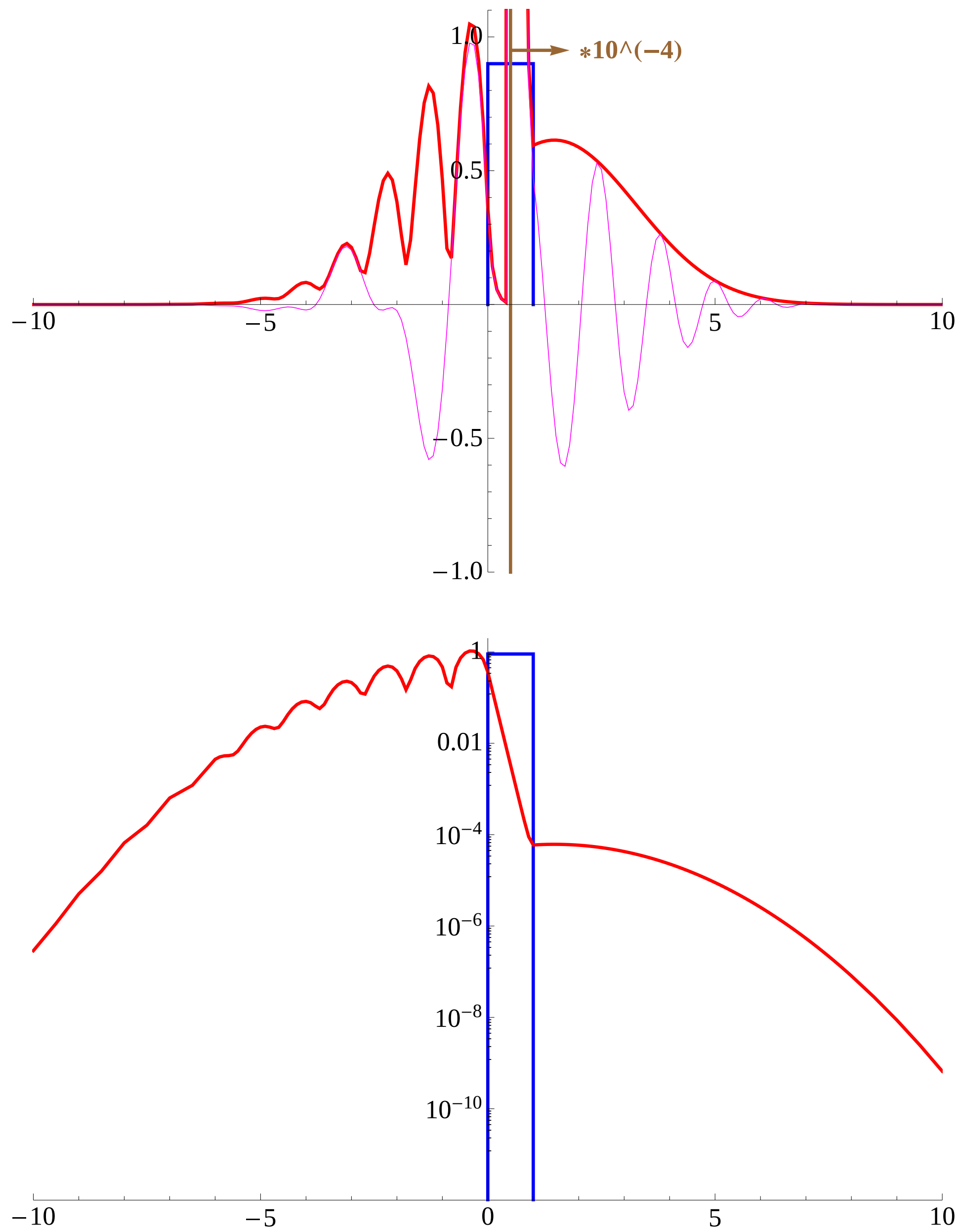


A: “Slow” wave packet, thin barrier

$t = 0.5$

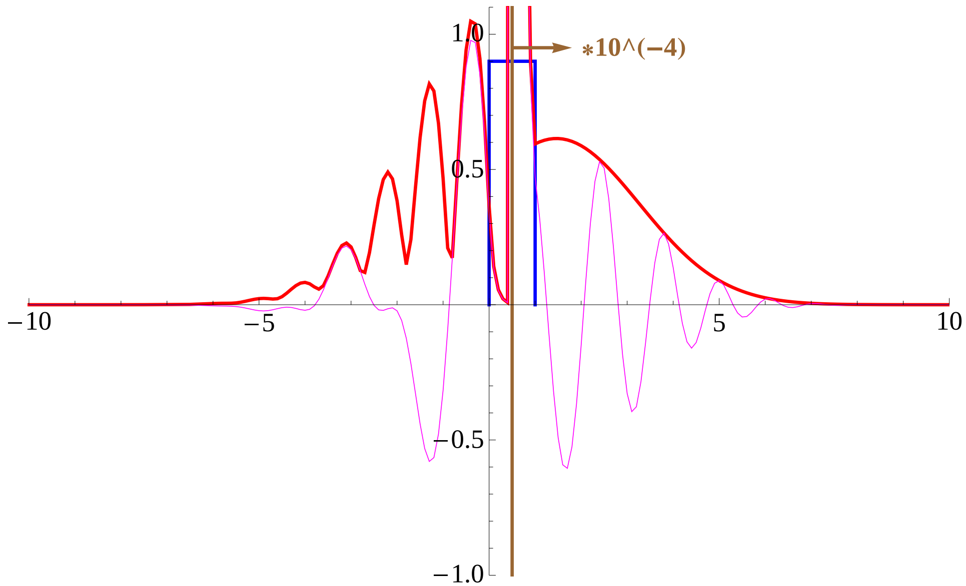


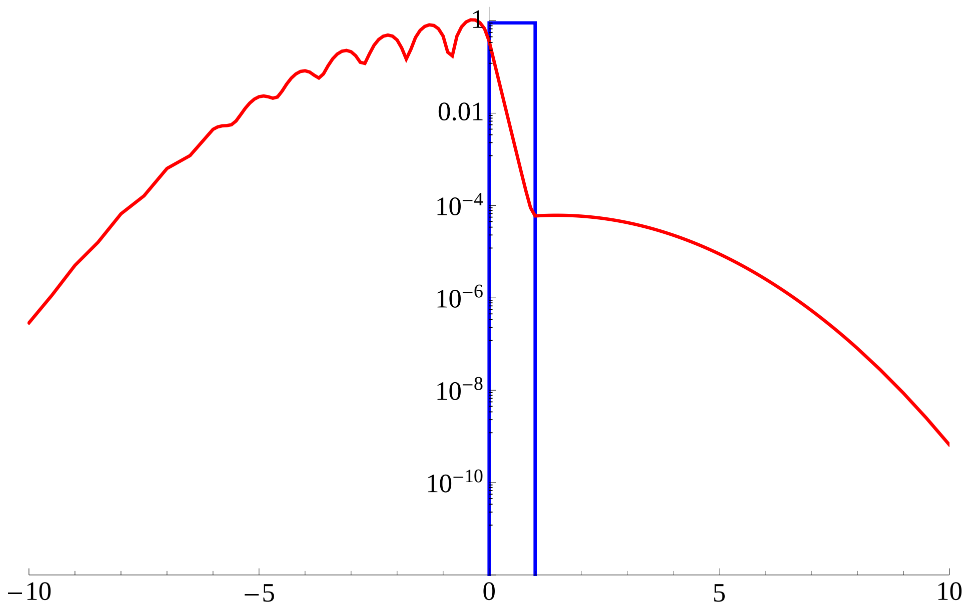
$t = 0.75$



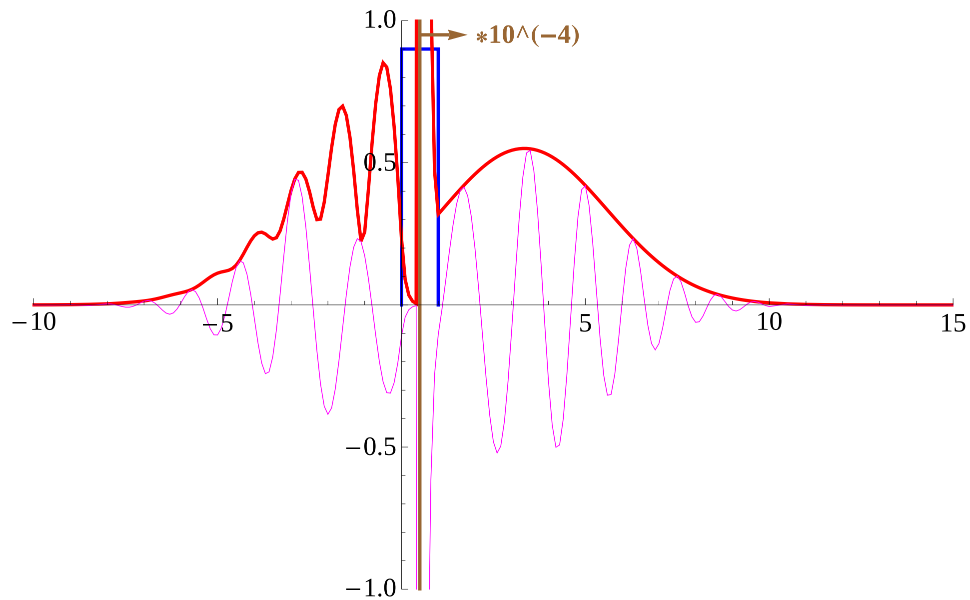
A: "Slow" wave packet, thin barrier

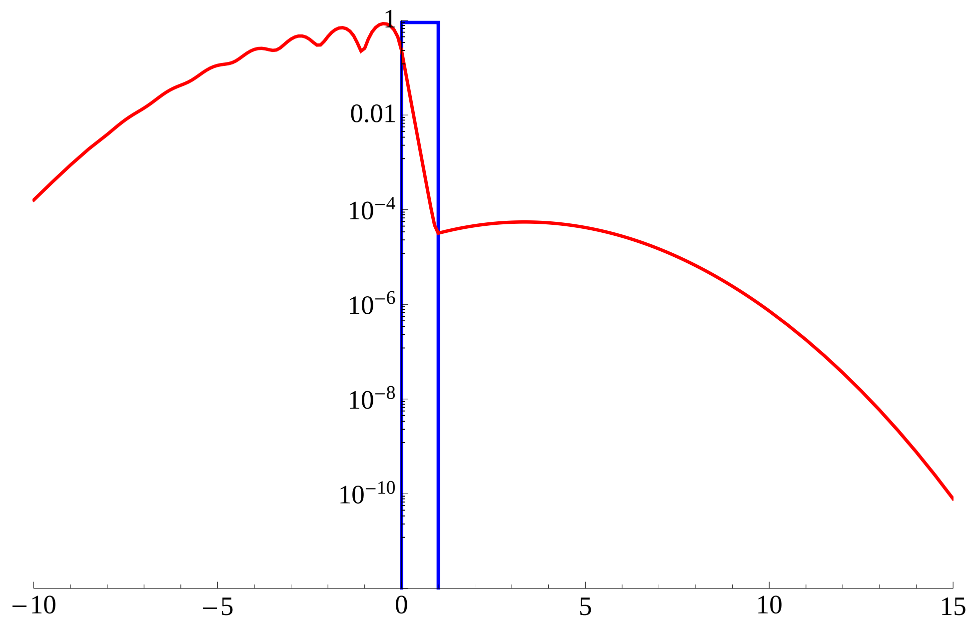
$t = 0.75$



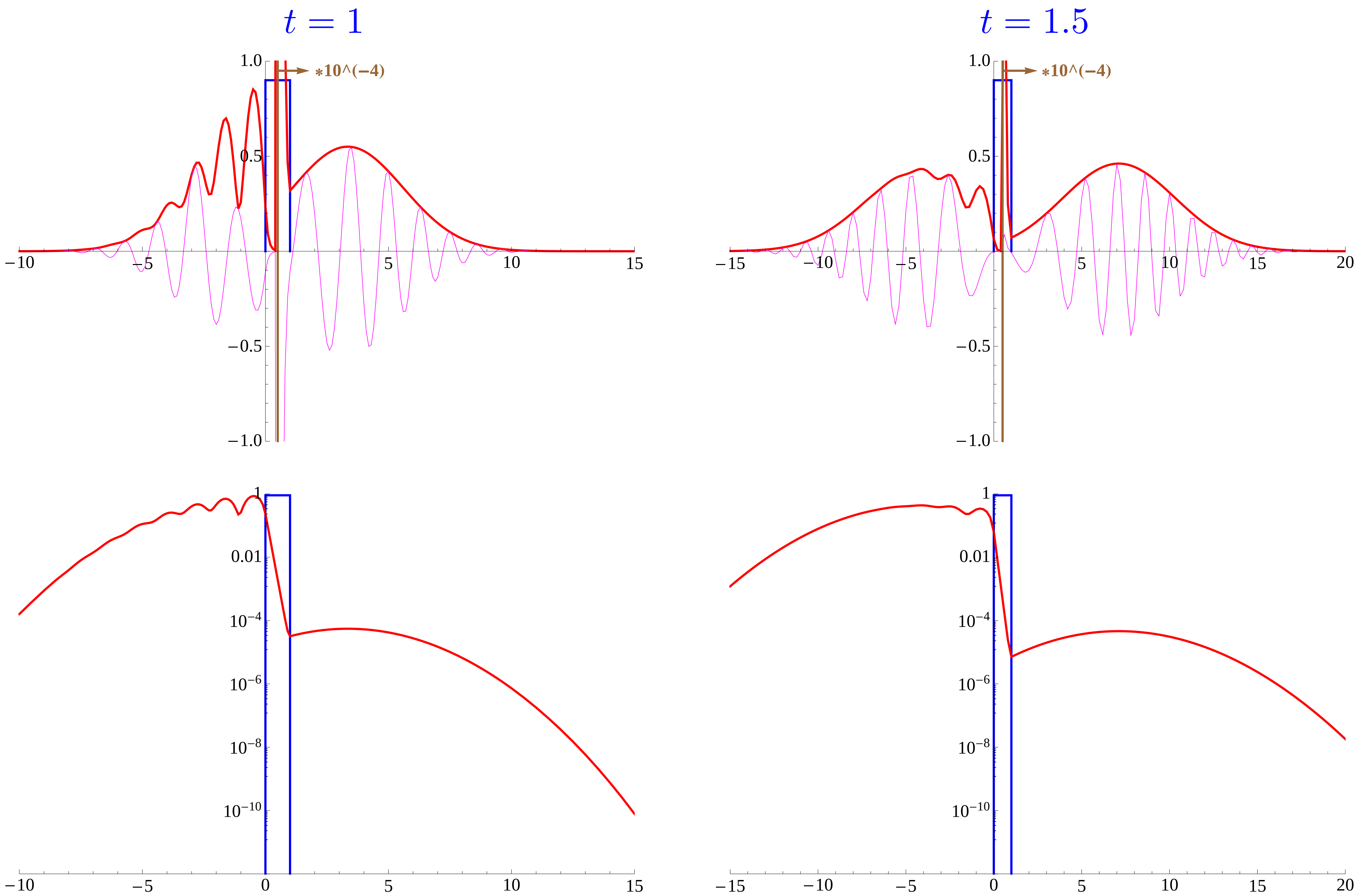


$t = 1$

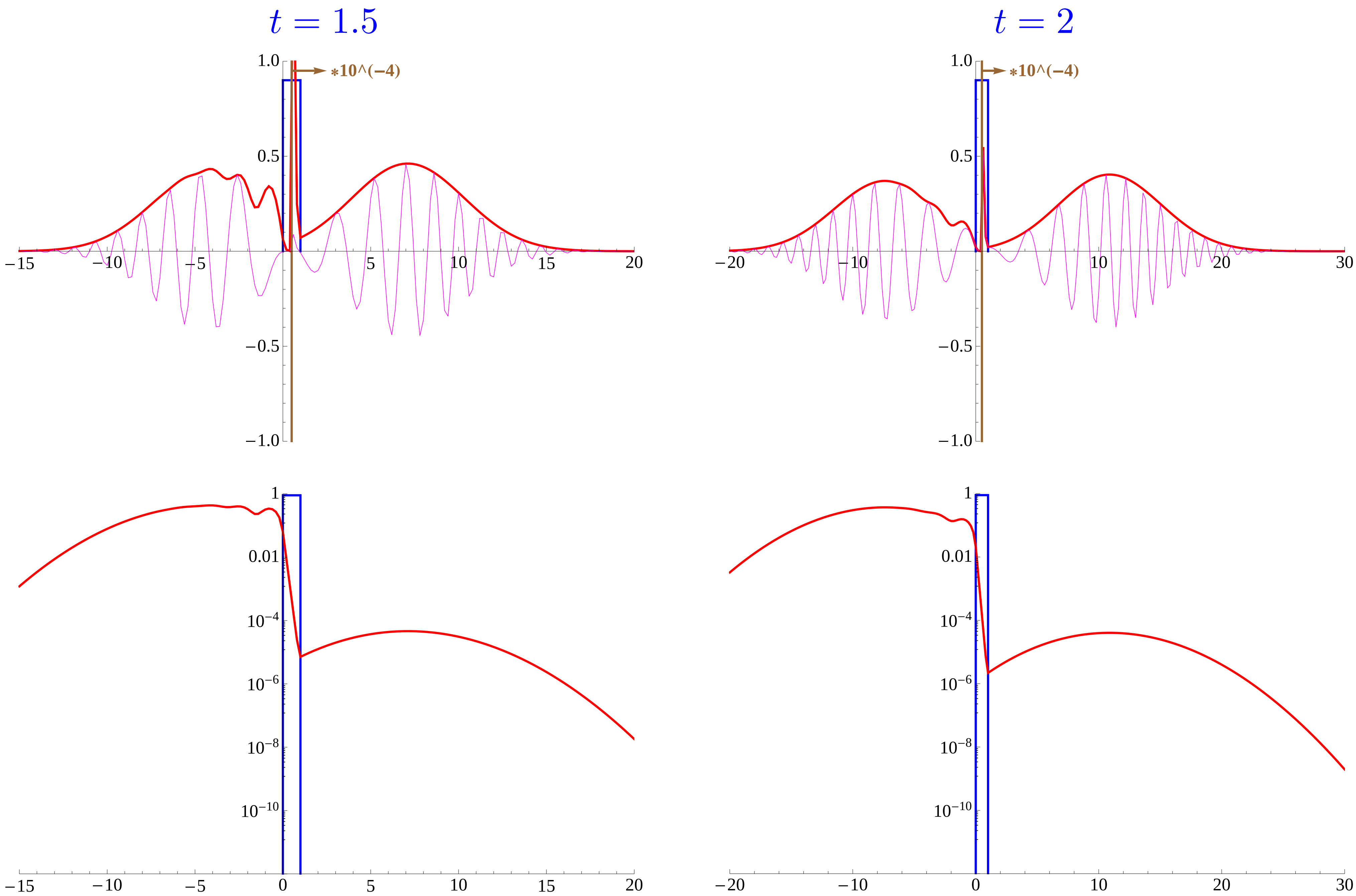




A: “Slow” wave packet, thin barrier

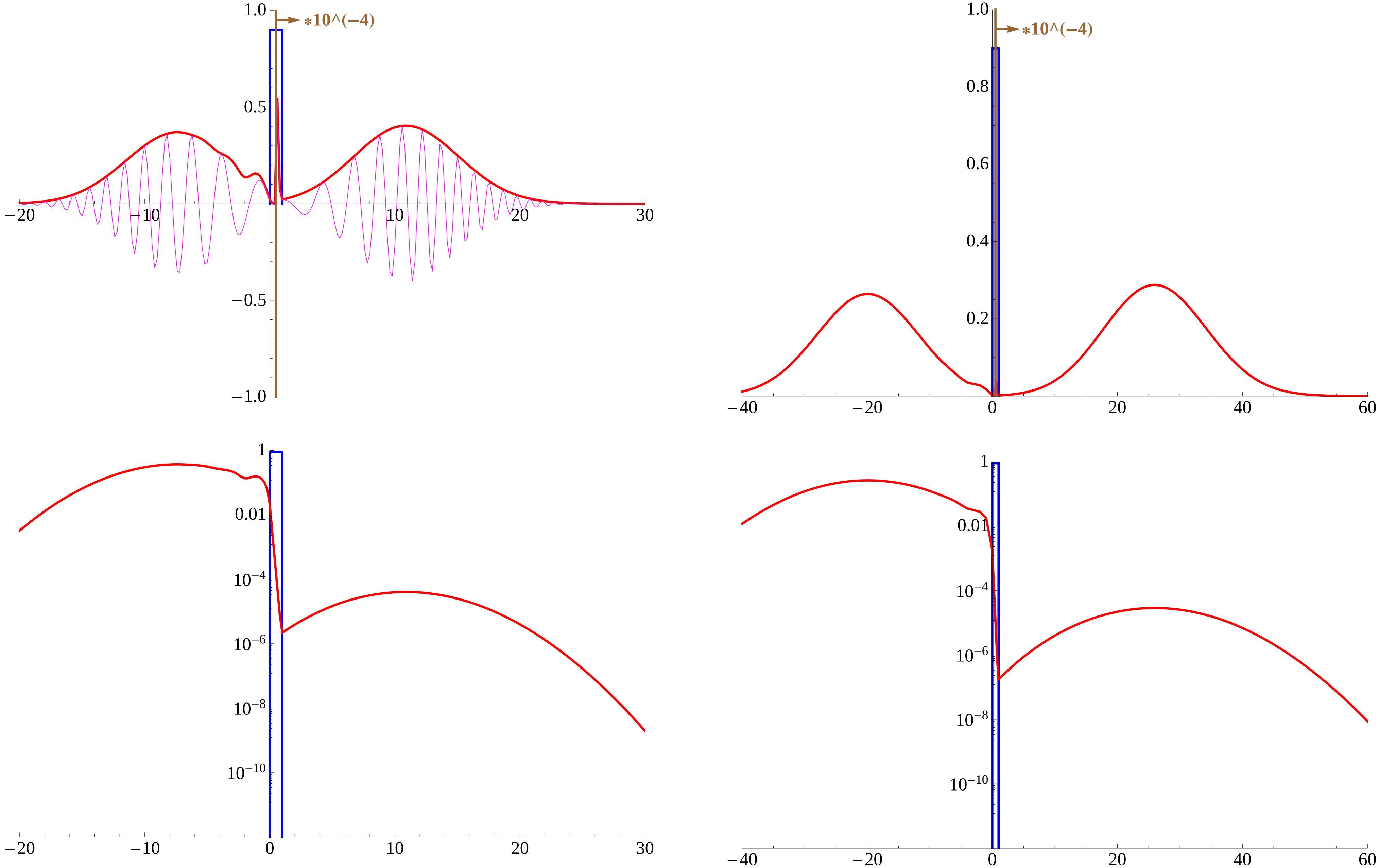


A: "Slow" wave packet, thin barrier

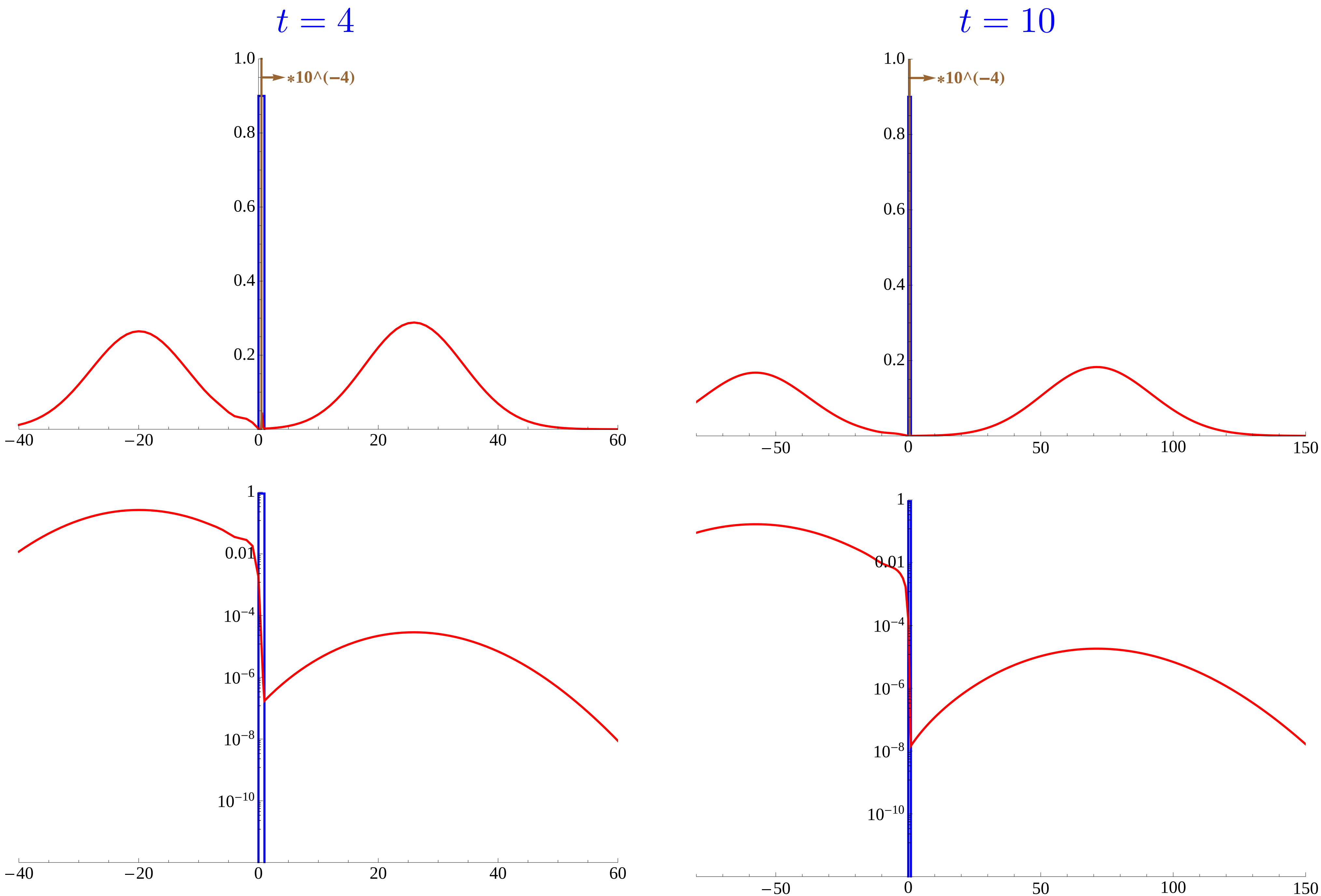


A: “Slow” wave packet, thin barrier

$t = 2$ $t = 4$



A: “Slow” wave packet, thin barrier



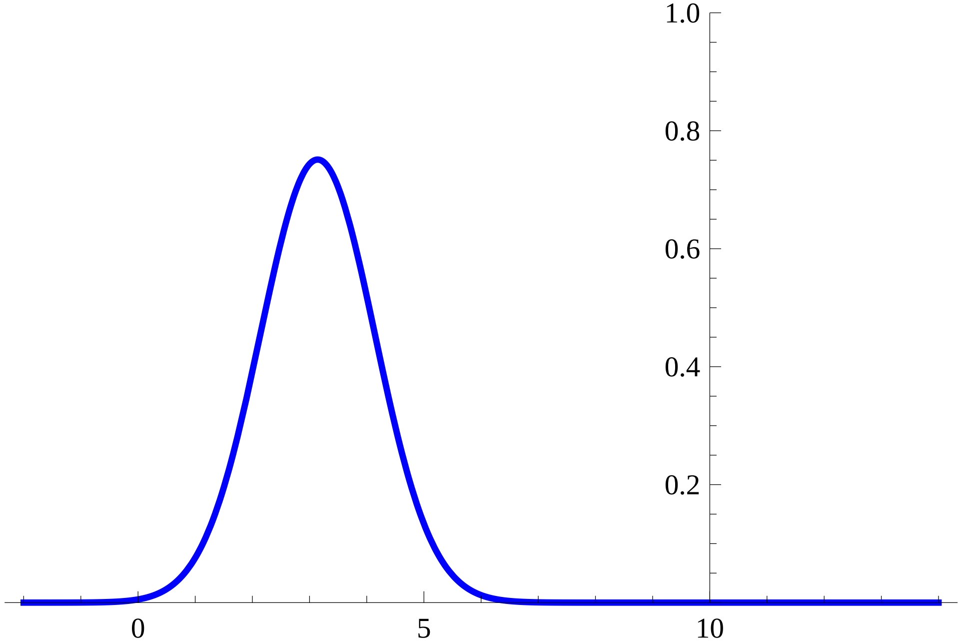
A: "Slow" wave packet, thin barrier — Conclusion

- Thin barrier: only modest exponential damping through the tunneling ($\sim 10^{-4}$)
  $\hookrightarrow$ transmission dominated by tunneling of low-momentum components.
- Incoming and reflected wave packet: wave length ($2\pi/k$) and velocity of maximum ($2k$) correspond to $k_0 = \pi$ and to a reflection at $x = 0$.
- In the tunnel: exponential decrease, no structure
- Transmitted wave packet: wave length $\rightsquigarrow k \approx 4$, velocity of maximum
  $\rightsquigarrow 3.5 \lesssim k \lesssim 4 \Rightarrow k \gtrsim k_0,\ k^2 \ll V$
- Packet maximum enters tunnel at $t = 0.8$ and exits at $t = 0.7$
  $\Rightarrow \Delta t_{\text{tunnel}} \approx -0.1 \lesssim 0$
- Reflected and transmitted wave packets are approximately Gaussian.
  Only while overlapping with the barrier, the incoming/reflected wave packet develops fringes ("standing wave").

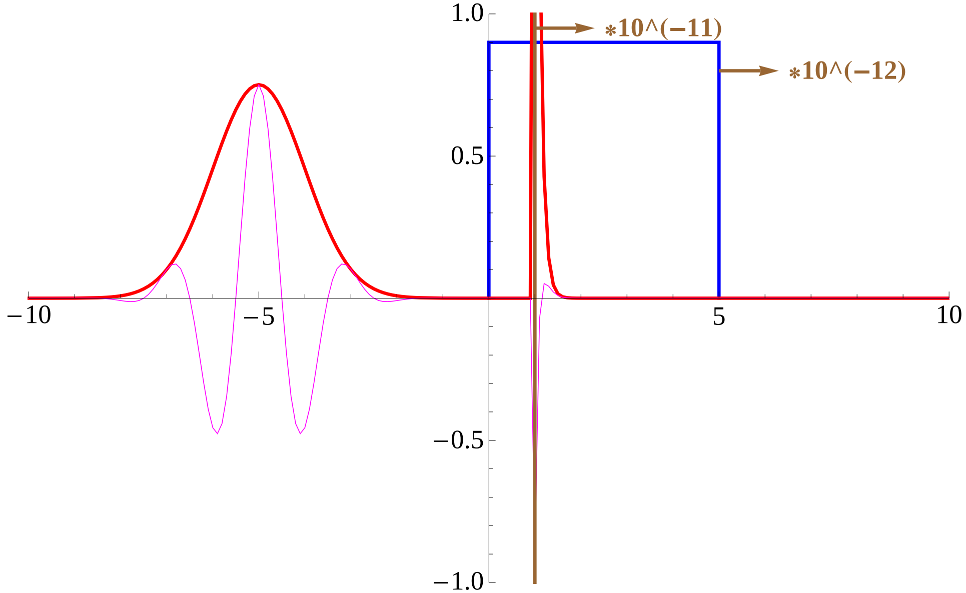
B: "Slow" wave packet, thick barrier

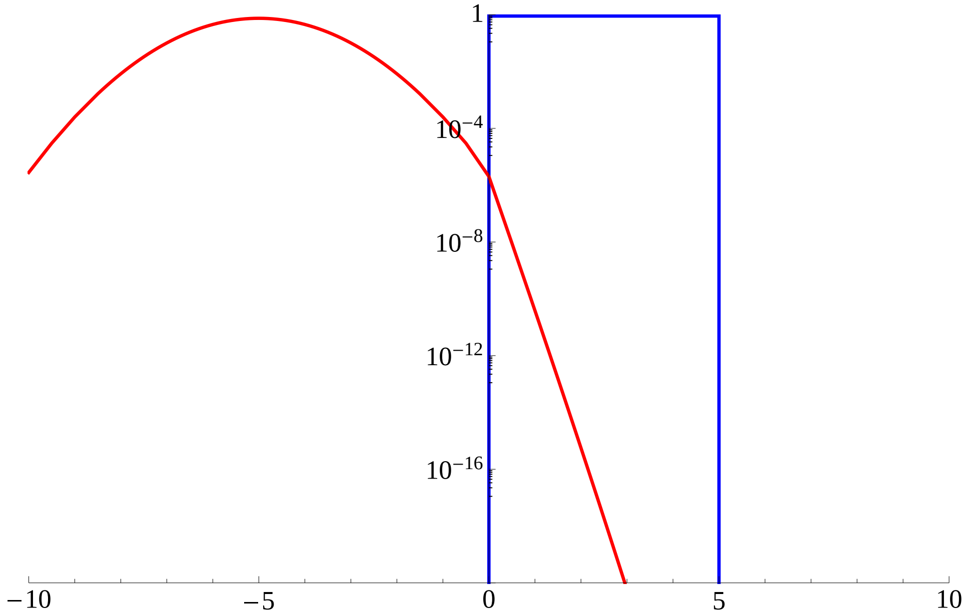
Parameters: $k_0 = \pi \gtrsim \sigma_k$,
$L = 5 > \{\sigma_x, \pi/k_0\}$, $\sigma_k = 1/\sqrt{2} \approx 0.7$,
$x_0 = -5$, $2m = 1$, $V = 10^2 \gg k_0^2$

Momentum distribution $|A(k)|$:



$t = 0$

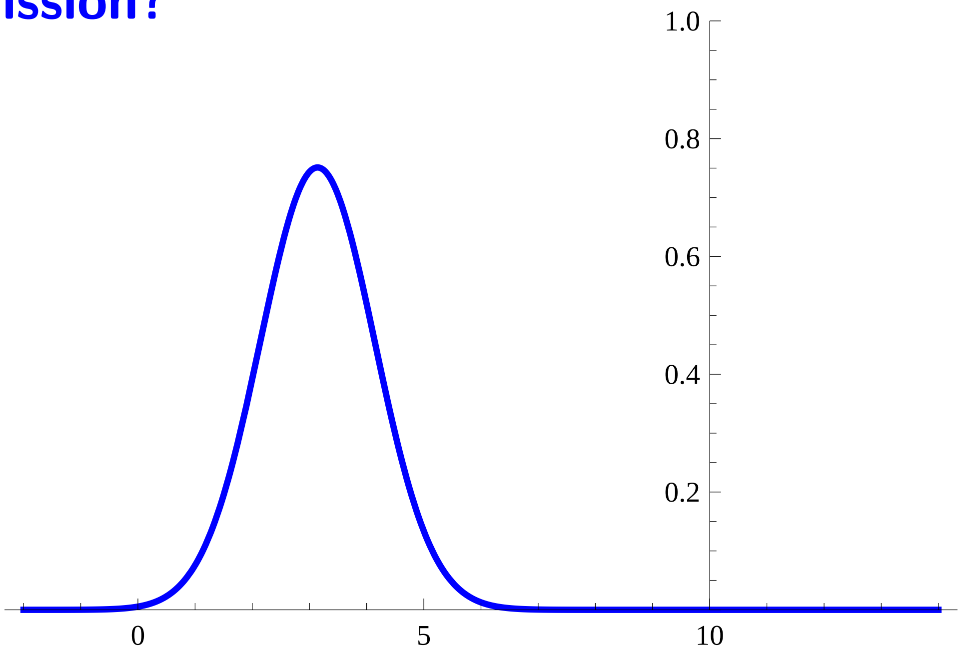




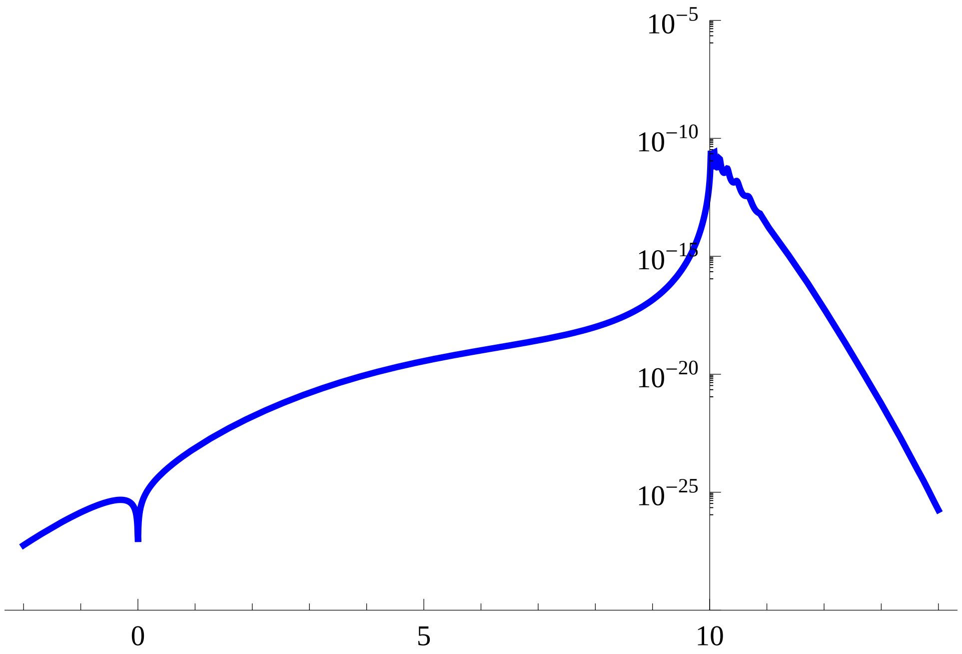
Right plots: barrier, $|\psi(t,x)|$, $\mathrm{Re}\,\psi(t,x)$;
top: to scale by 10^{-11} for $1 < x < L$
and by 10^{-12} for $x > L$;

B: "Slow" wave packet, thick barrier — Which momenta contribute to the transmission?

Momentum distribution of incoming wave packet, i.e. part of $\tilde{\psi}(k;t,x) \propto e^{ikx}$ at $x < 0$: $|A(k)|$



Momentum distribution of transmitted wave packet, i.e. $\tilde{\psi}(k;t,x)$ at $x > L$: $|A(k)\,\tilde{\psi}(k;t,L)|$ (logarithmic scale)

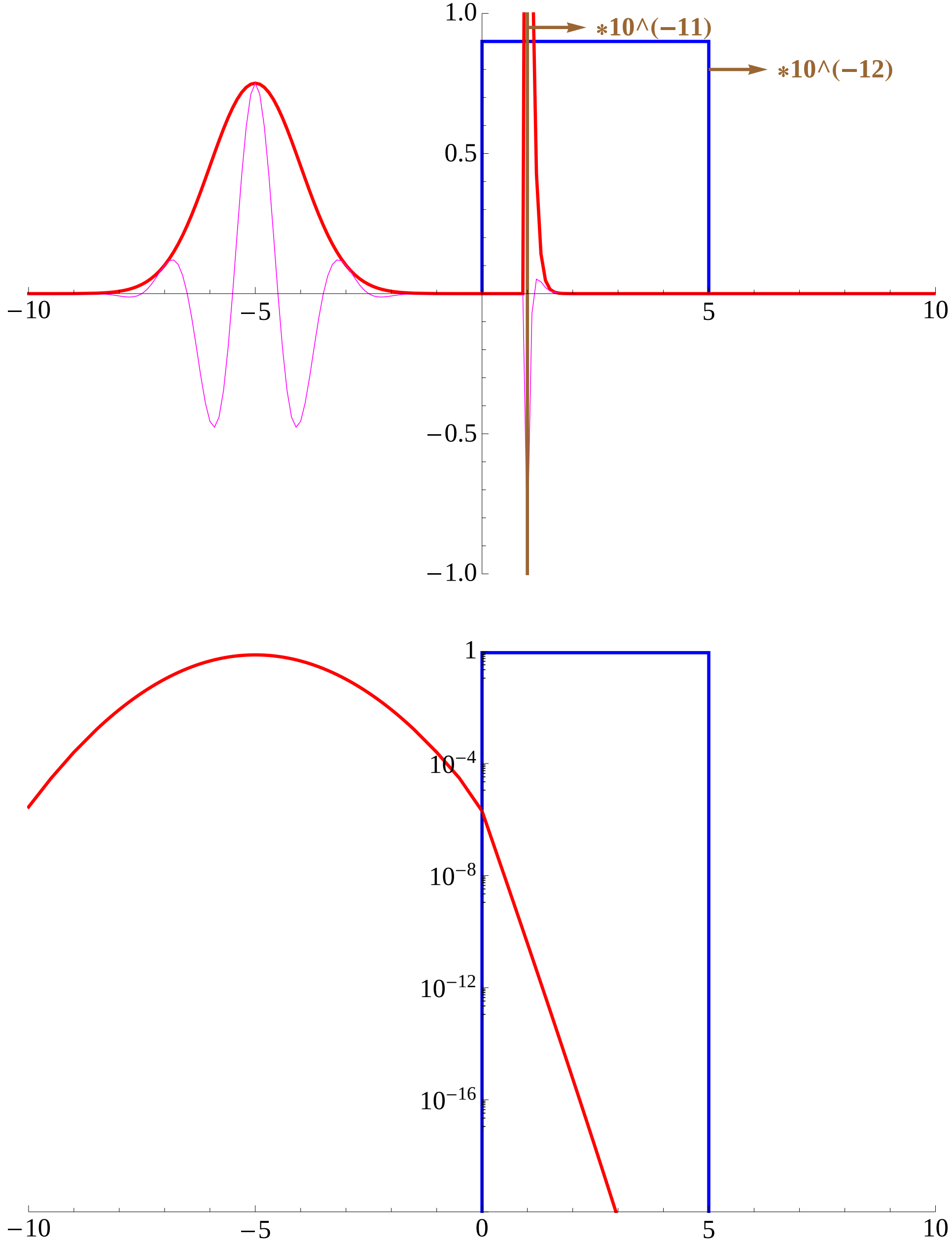


$\Rightarrow$ transmission dominated by high momenta $k \gtrsim \sqrt{V}$

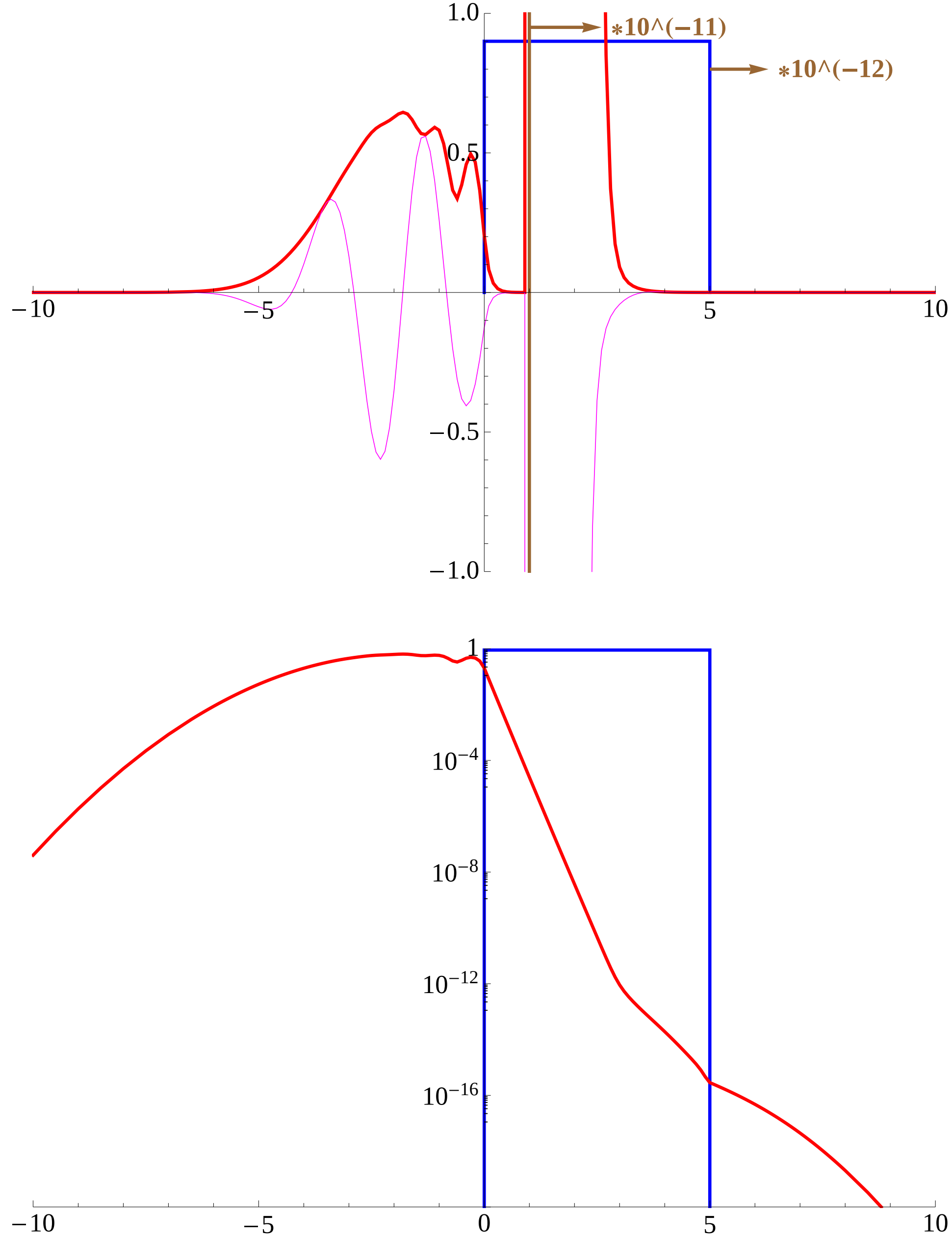
$\Rightarrow$ classically allowed transmission

B: "Slow" wave packet, thick barrier

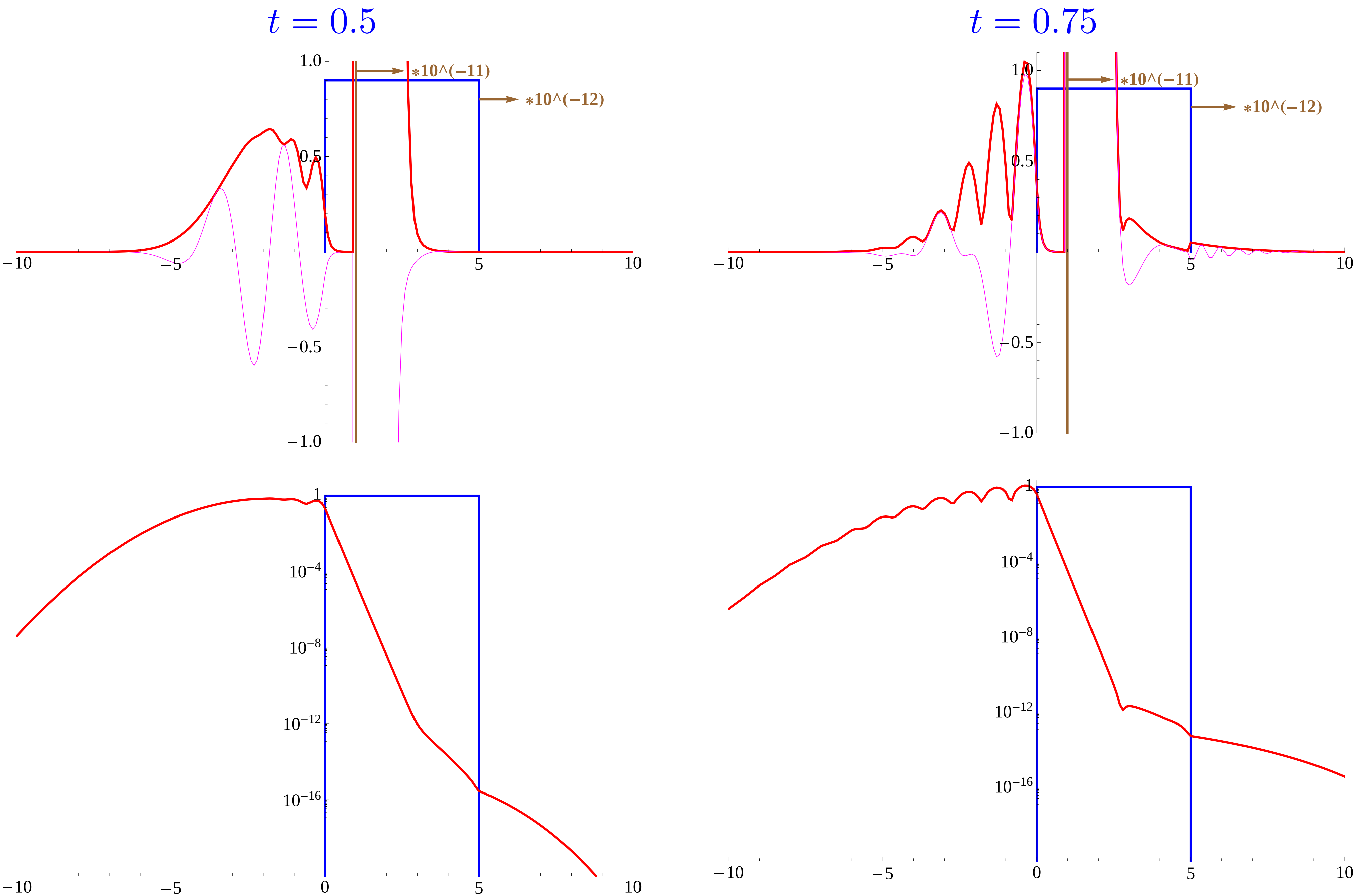
$t = 0$



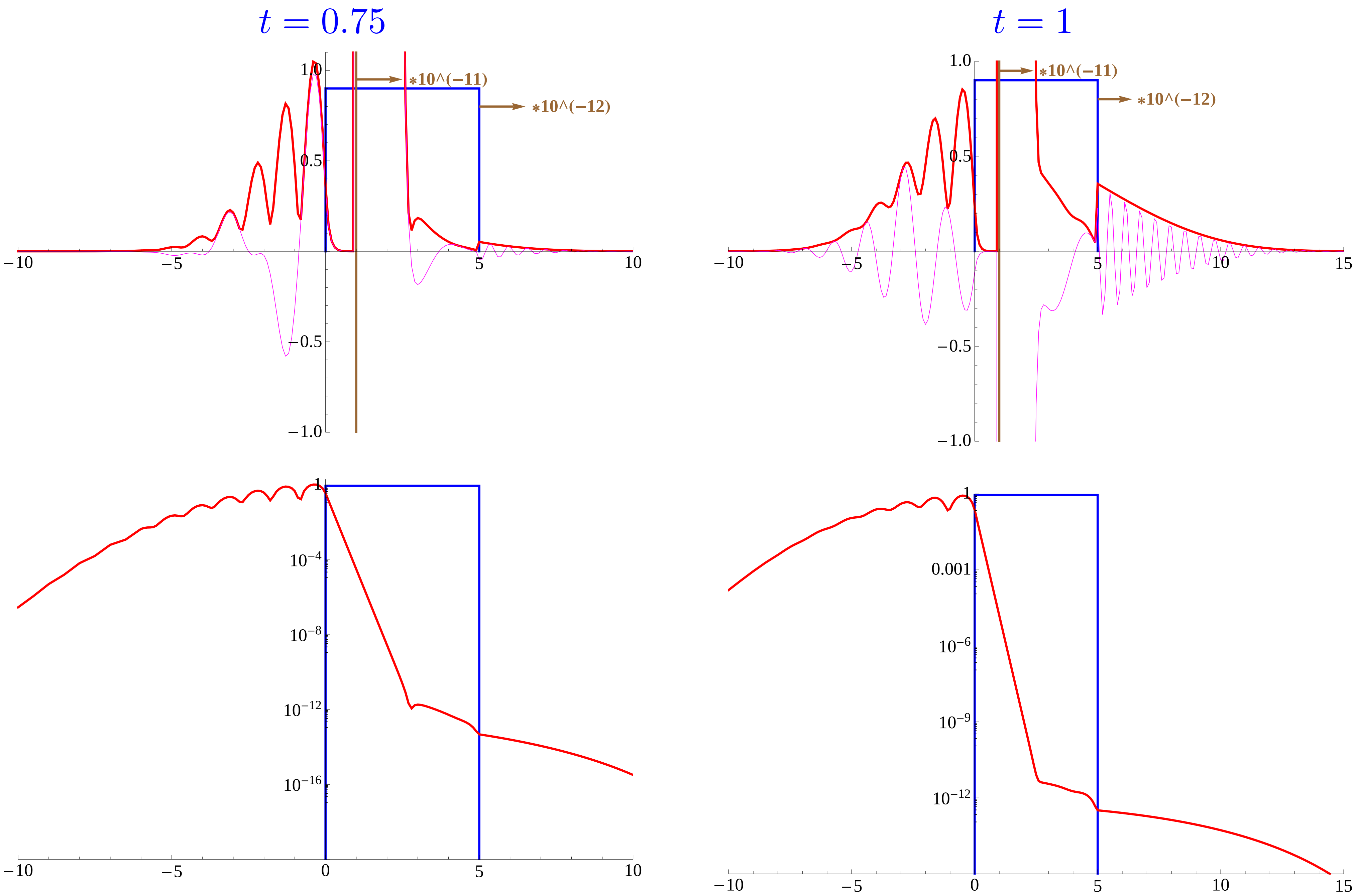
$t = 0.5$



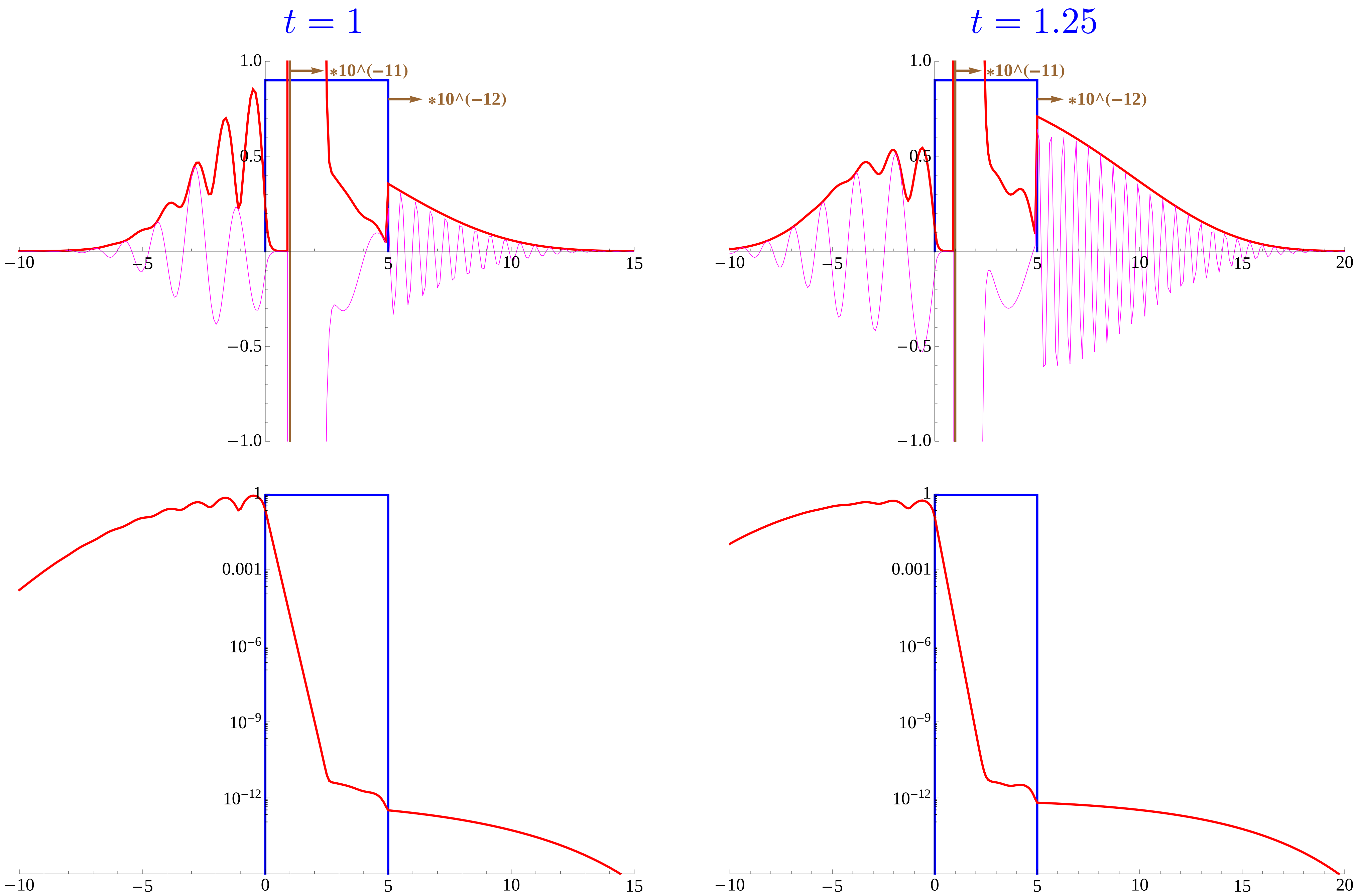
B: "Slow" wave packet, thick barrier



B: “Slow” wave packet, thick barrier

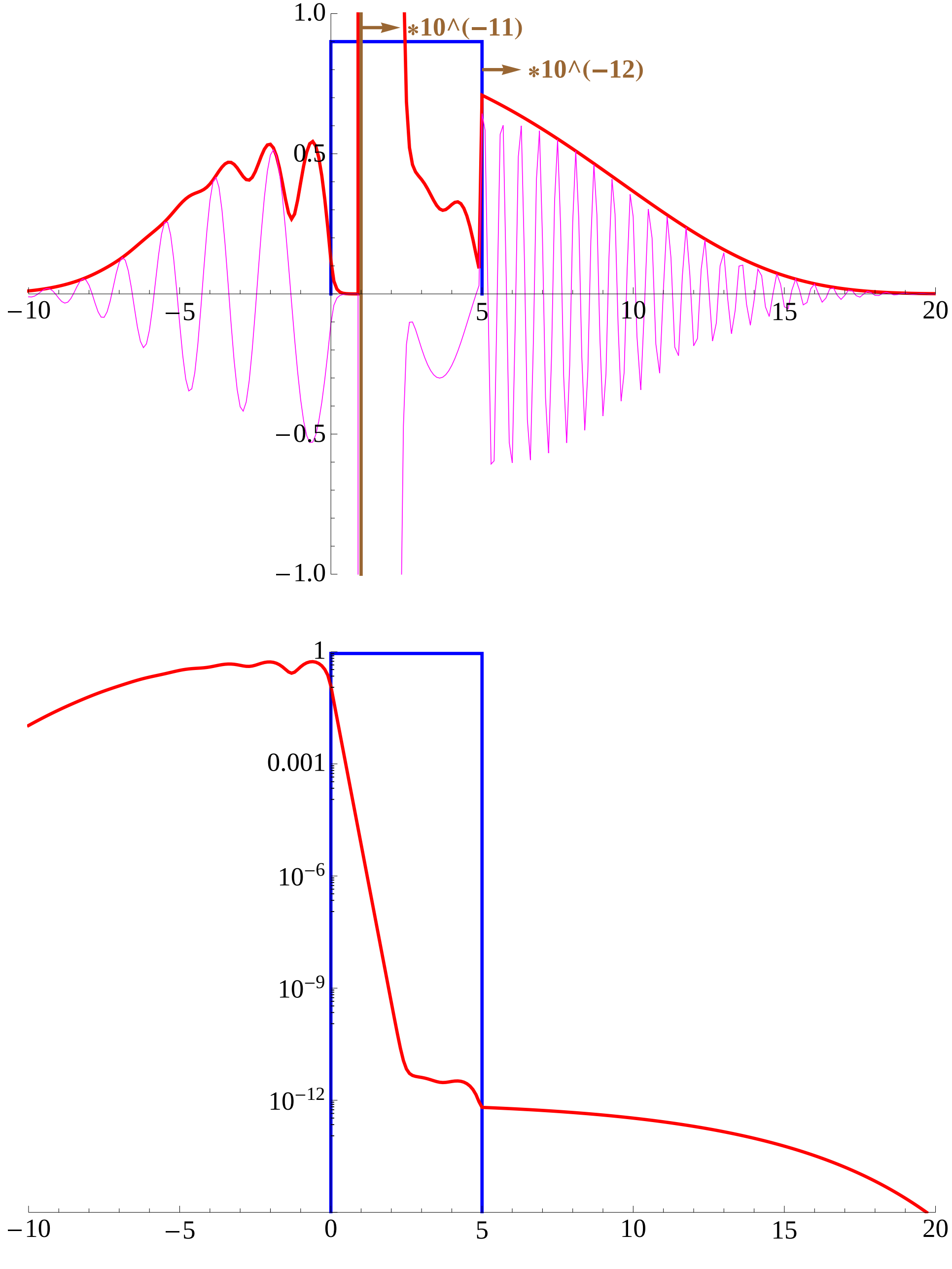


B: "Slow" wave packet, thick barrier

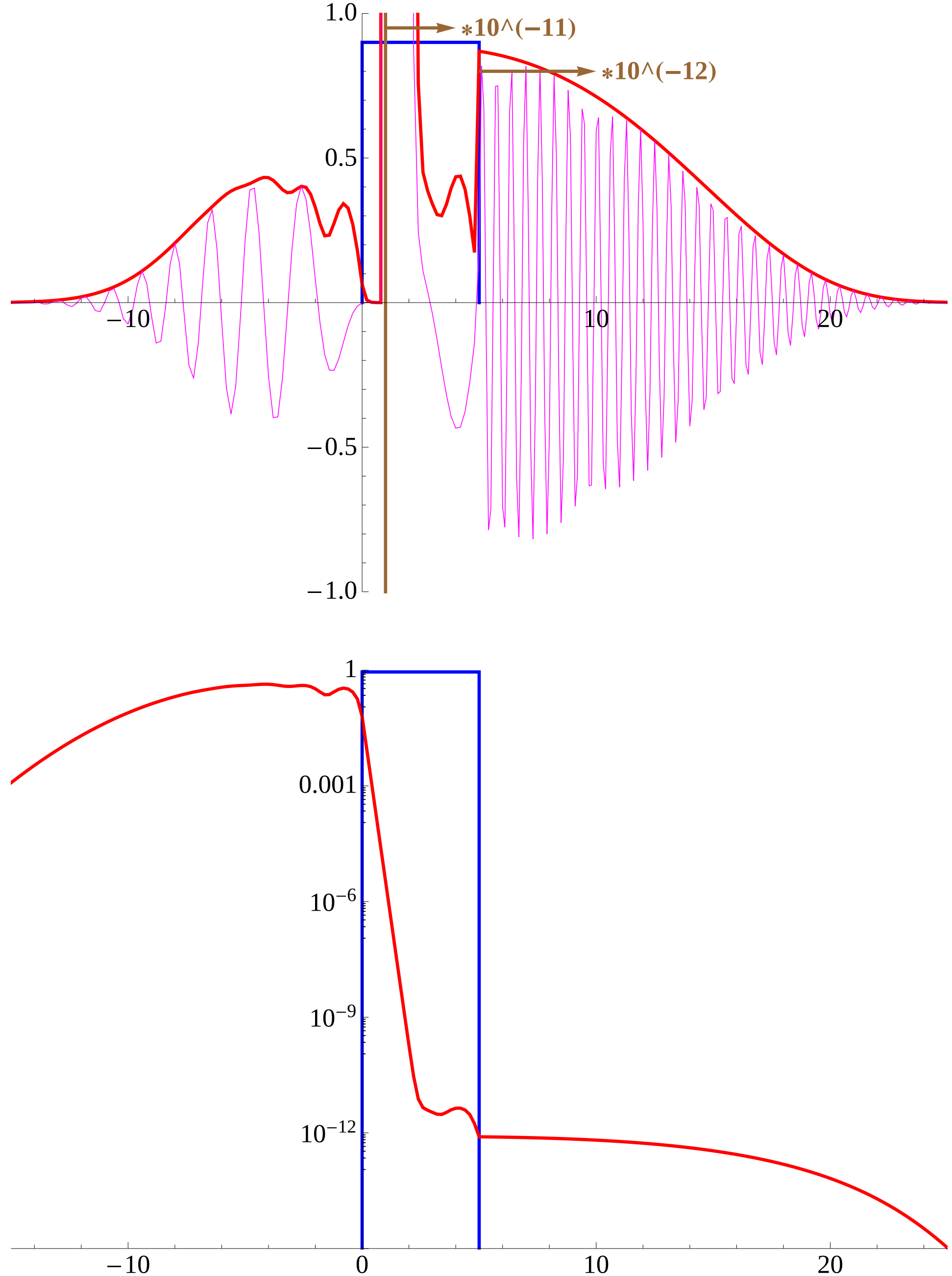


B: “Slow” wave packet, thick barrier

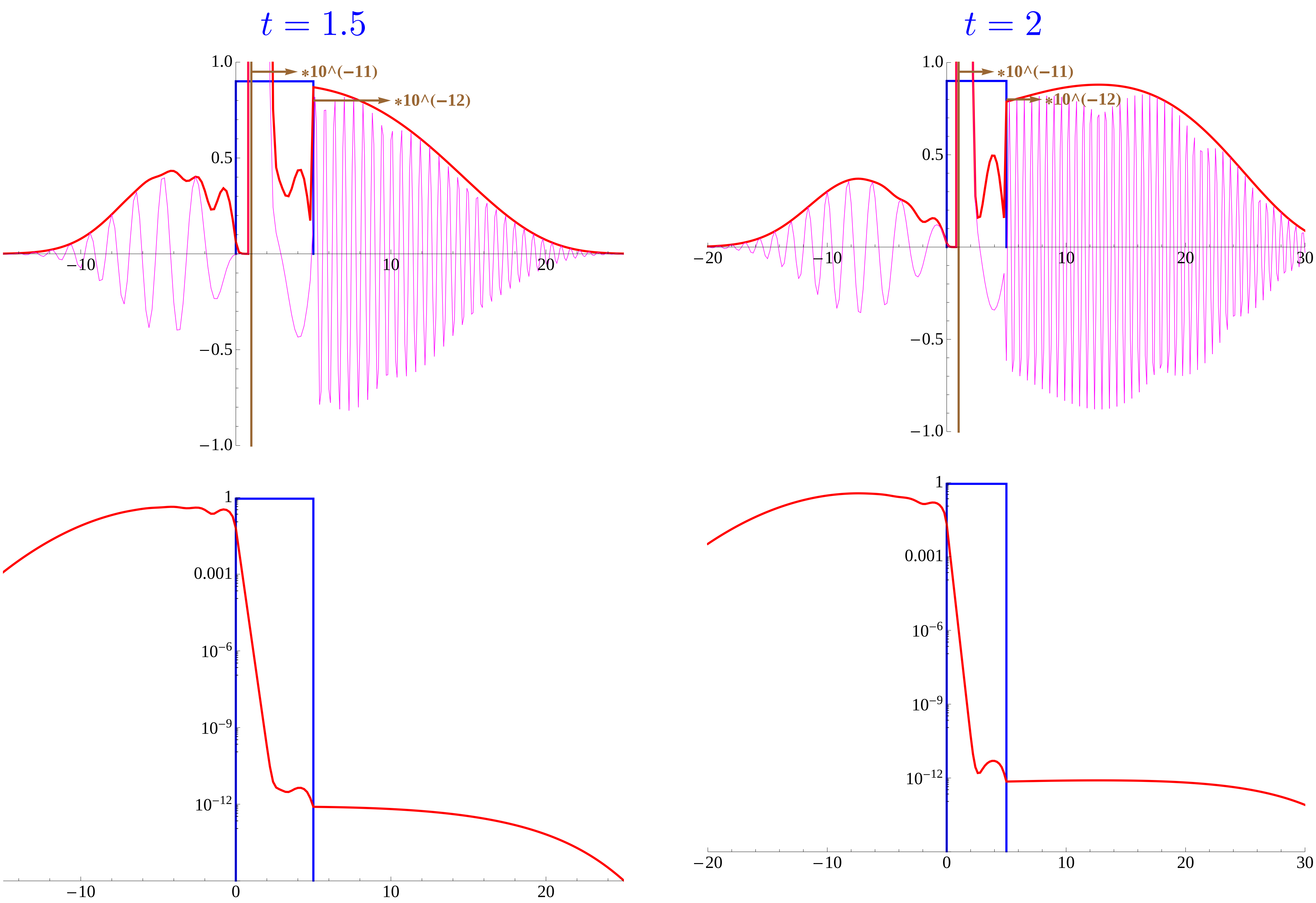
$t = 1.25$



$t = 1.5$

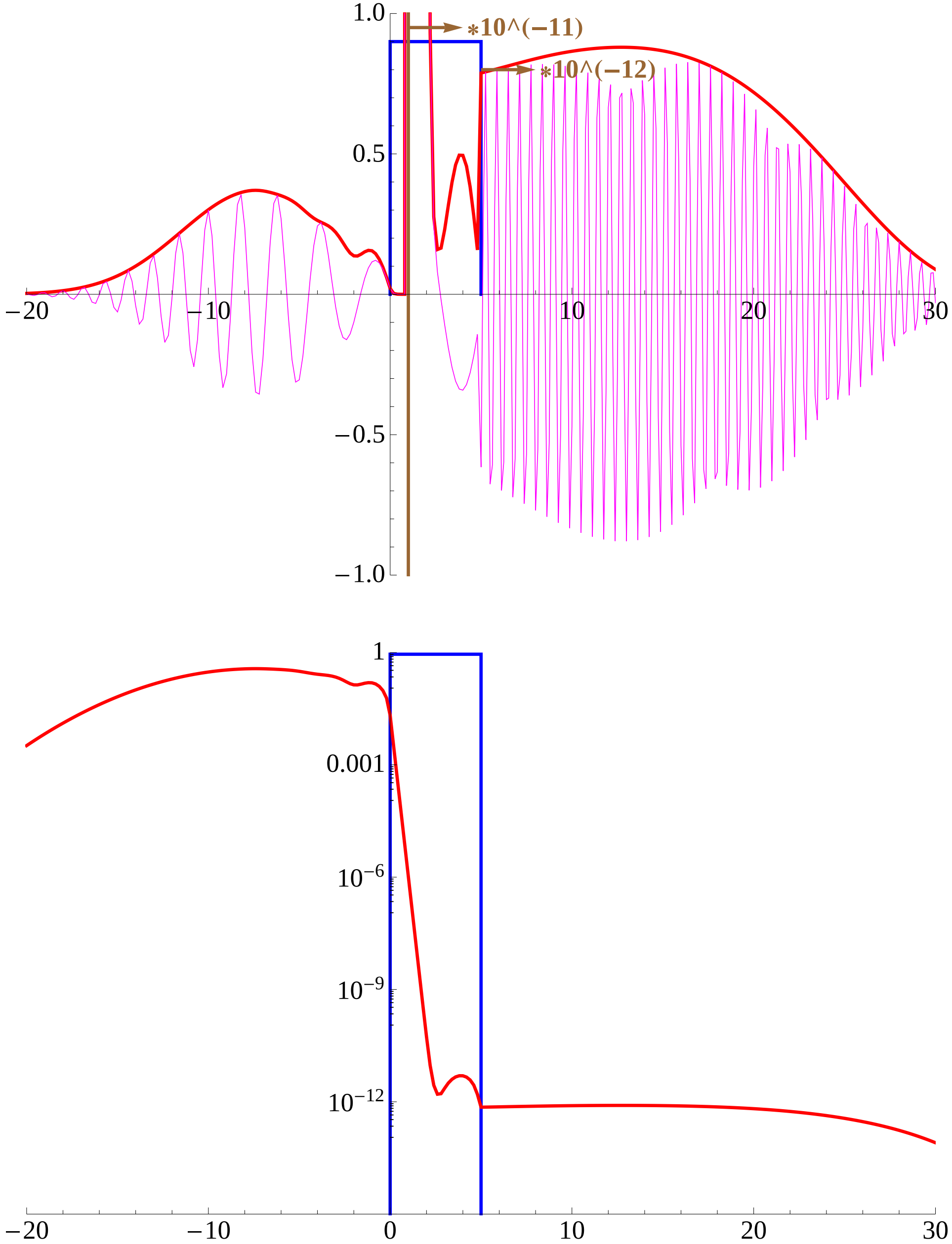


B: “Slow” wave packet, thick barrier

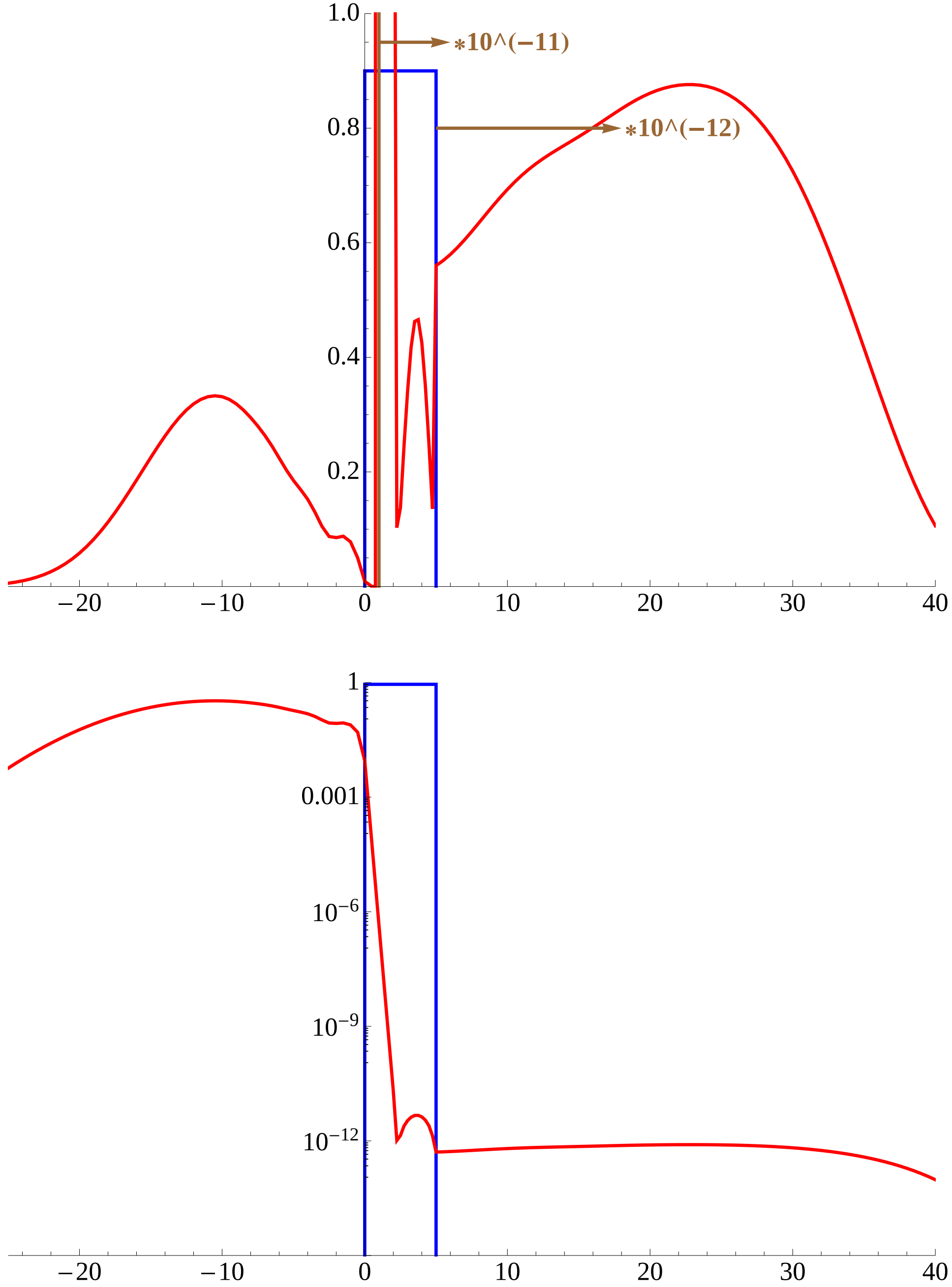


B: “Slow” wave packet, thick barrier

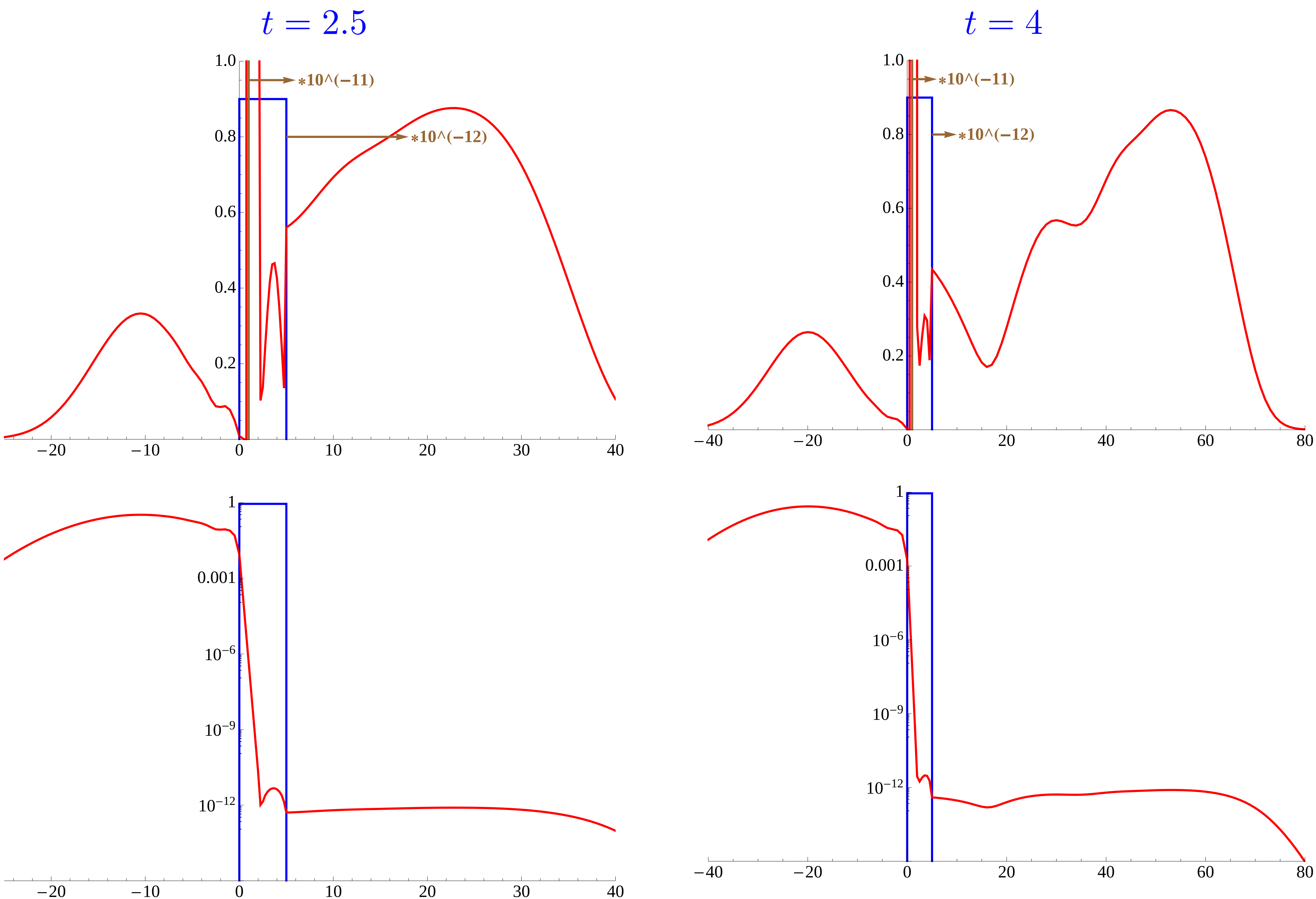
$t = 2$



$t = 2.5$

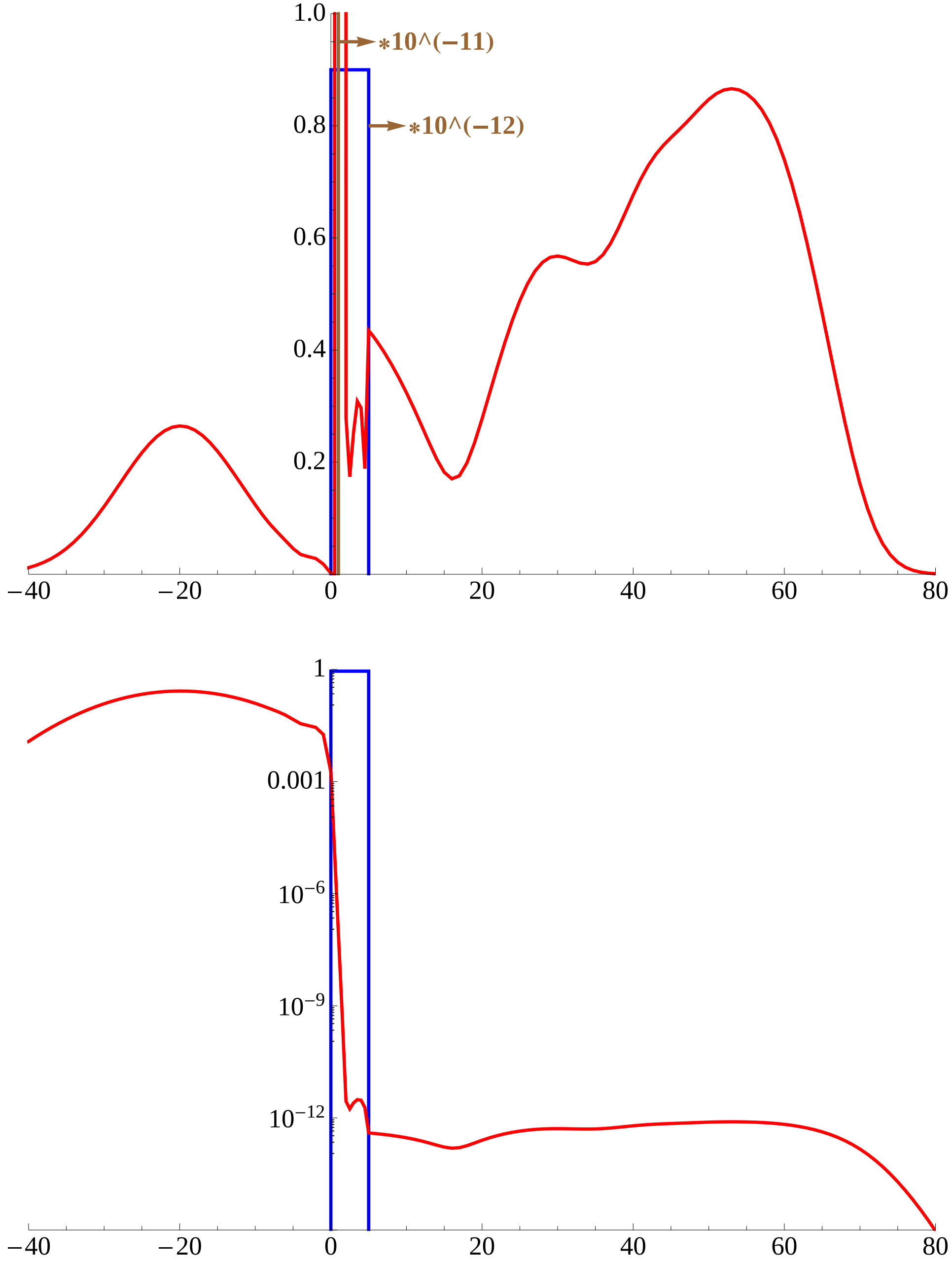


B: "Slow" wave packet, thick barrier

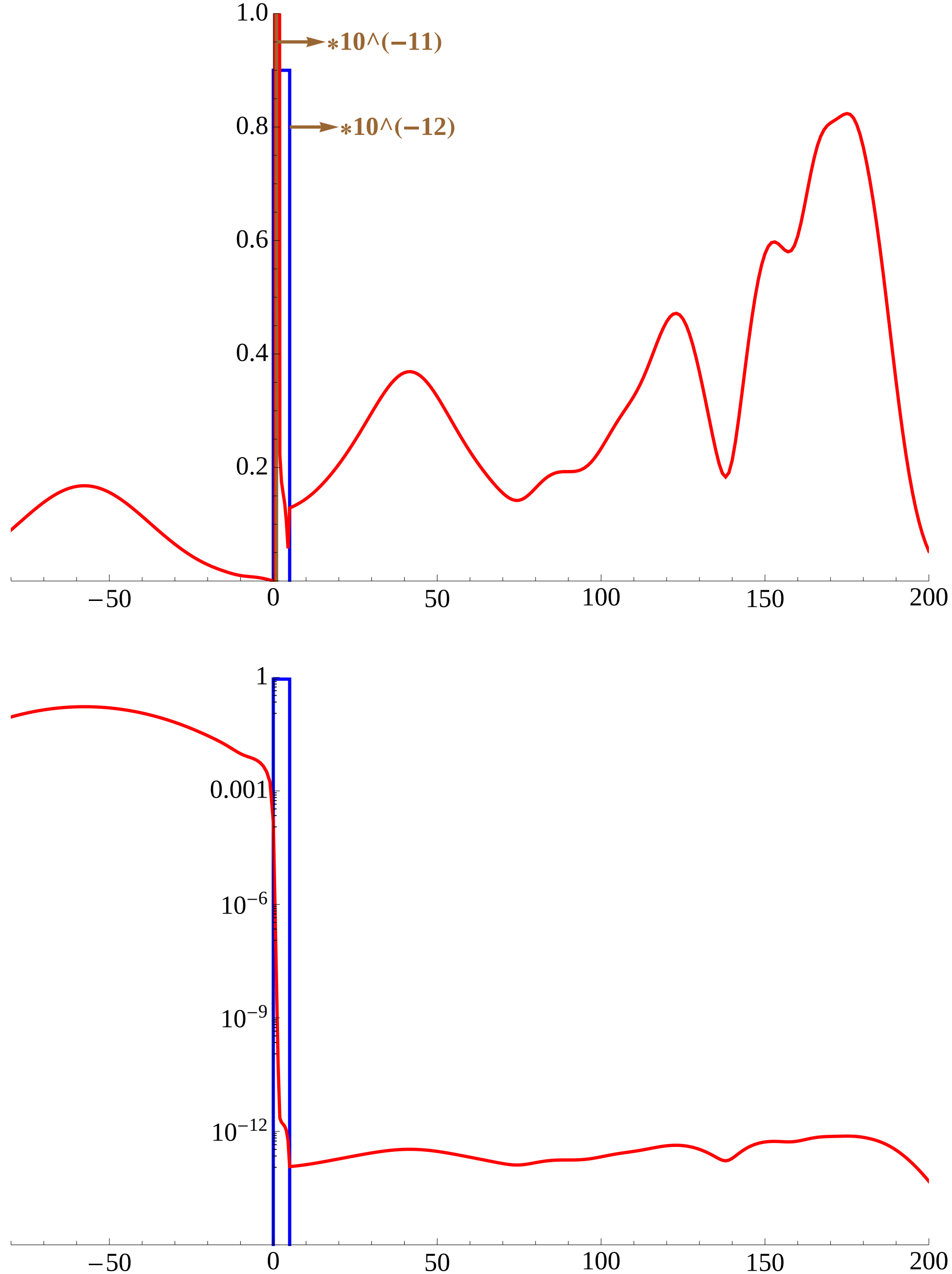


B: "Slow" wave packet, thick barrier

$t = 4$

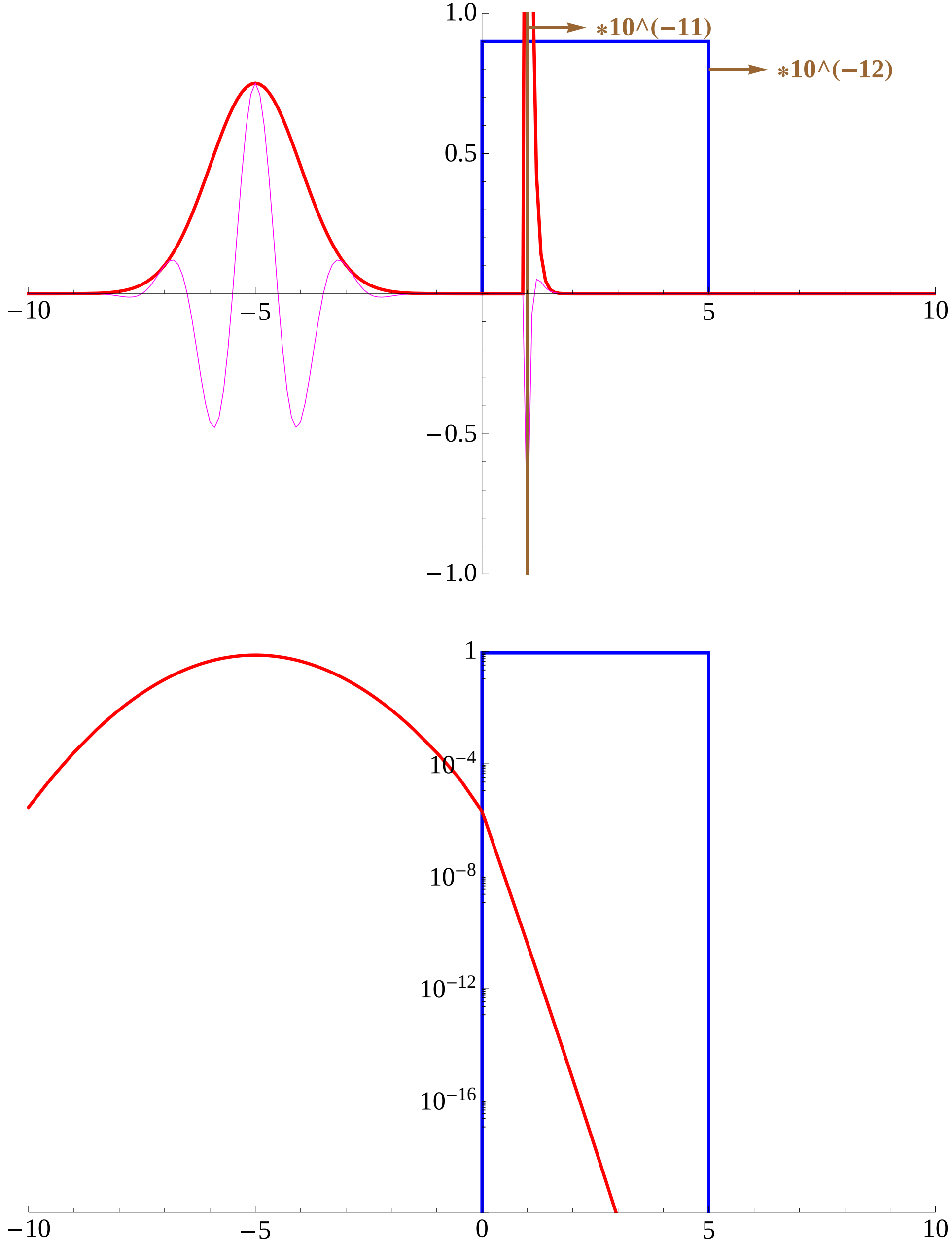


$t = 10$

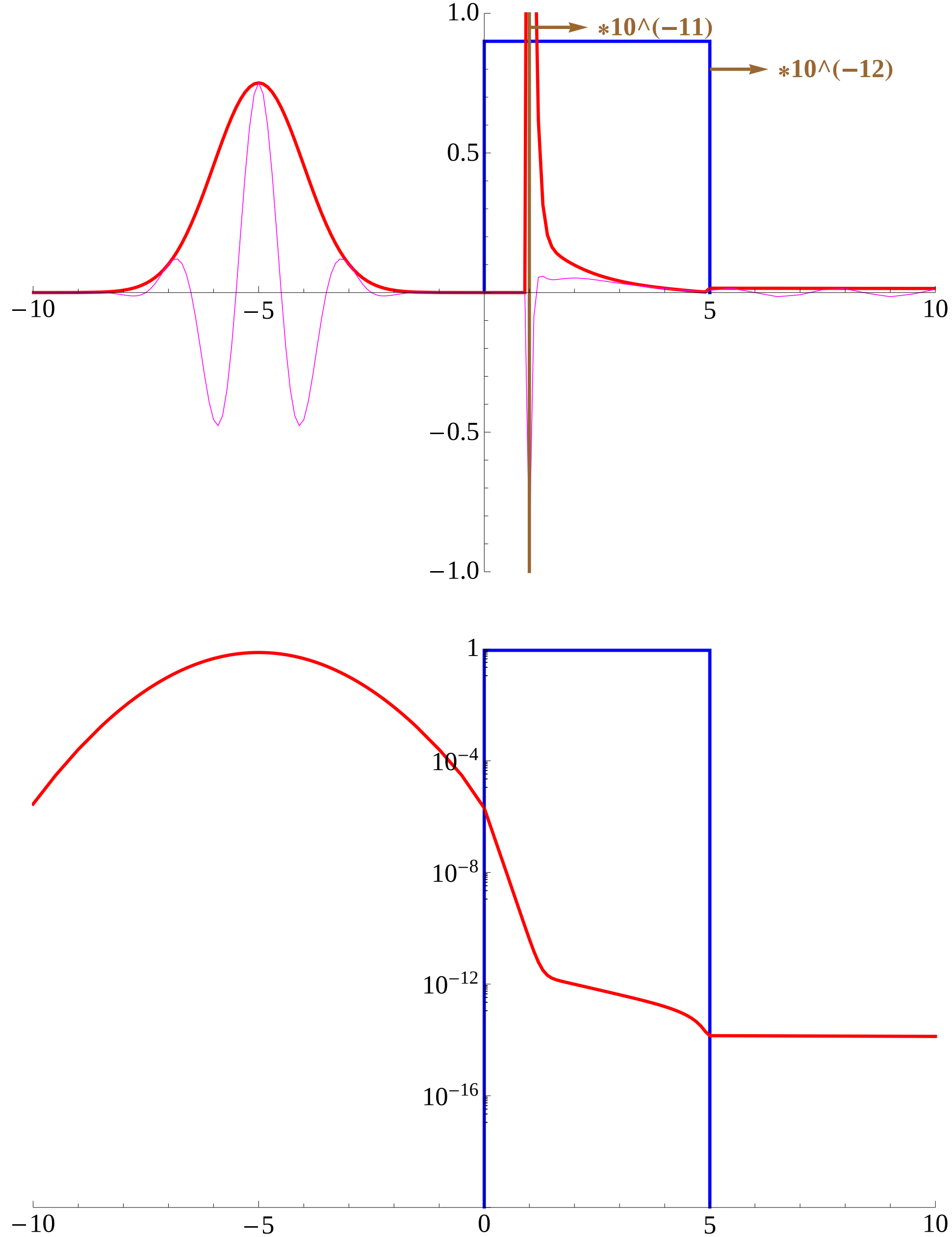


B: “Slow” wave packet, thick barrier — omitting high momenta

$t = 0$

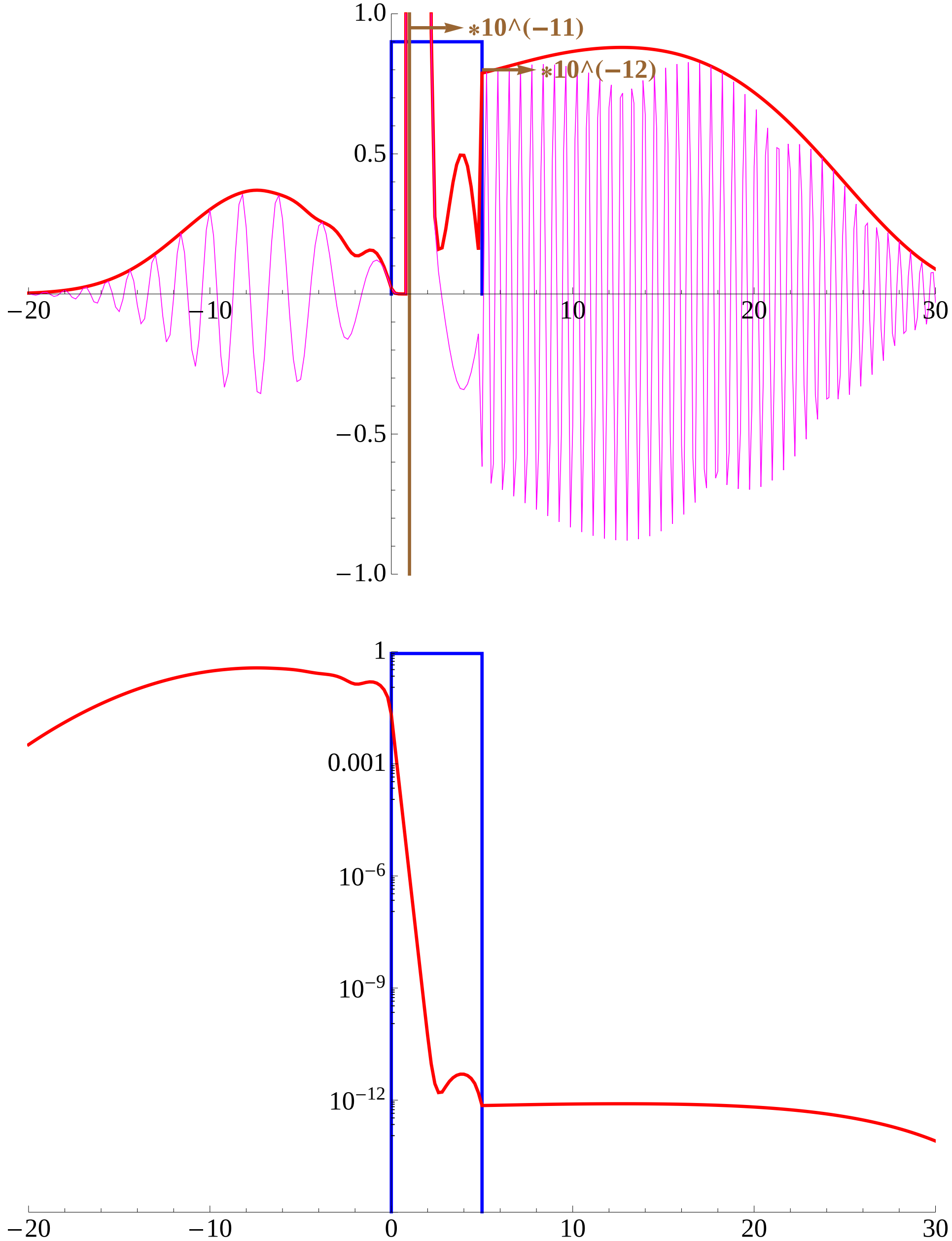


$t = 0$, with $k \leq \sqrt{V}$

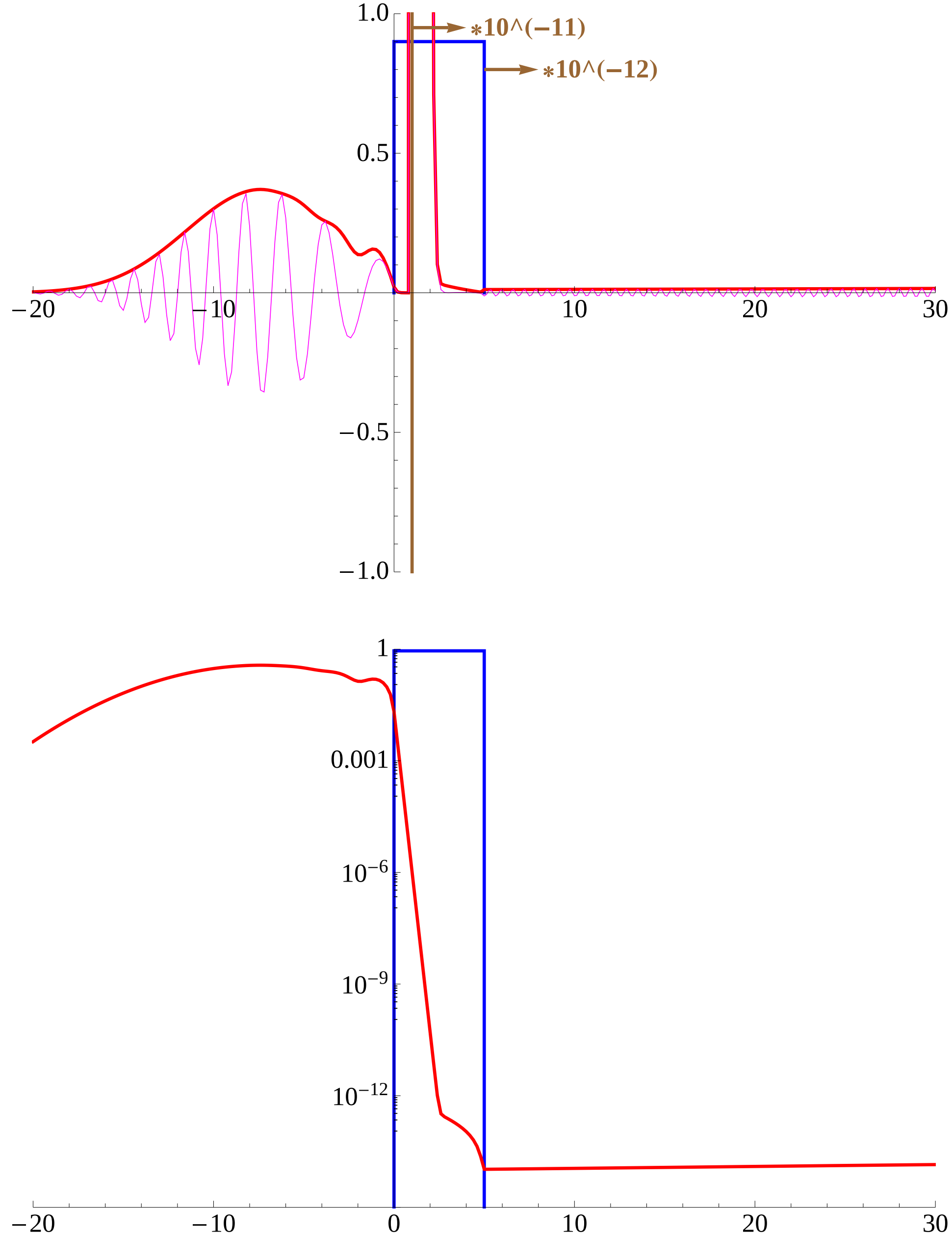


B: "Slow" wave packet, thick barrier — omitting high momenta (2)

$t = 2$



$t = 2$, with $k \leq \sqrt{V}$



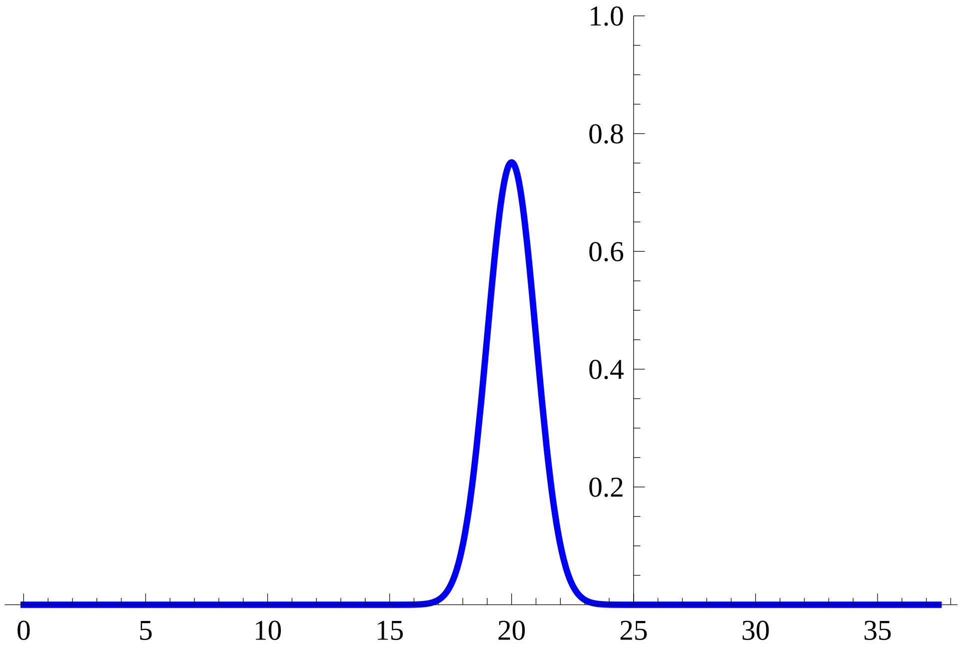
B: “Slow” wave packet, thick barrier — Conclusion

- Thick barrier: strong exponential damping through the tunneling ($\sim 10^{-20}$ at k_0)
  $\hookrightarrow$ dominated by classically allowed transmission of high momenta ($\sim 10^{-11}$).
- Incoming and reflected wave packet: like in case A – wave length and velocity of maximum correspond to $k_0 = \pi$ and to a reflection at $x = 0$.
- In the tunnel: structure appears (ankle, local maximum)
- Transmitted wave packet: wave length and velocity of maximum
  $\rightsquigarrow k \approx 10 = \sqrt{V} \gg k_0$
- Omitting high momenta $k > \sqrt{V}$ in integration:
  no transmission from low momenta
- Packet maximum enters tunnel at $t = 0.8$ and exits at $t = 1.6$
  $\Rightarrow \Delta t_{\text{tunnel}} \approx 0.8 > 0$ ($v_{\text{tunnel}} = L/\Delta t_{\text{tunnel}} \approx 2\pi \rightsquigarrow k_{\text{tunnel}} \approx k_0$)
- Transmitted wave packet develops tail of lower maxima.

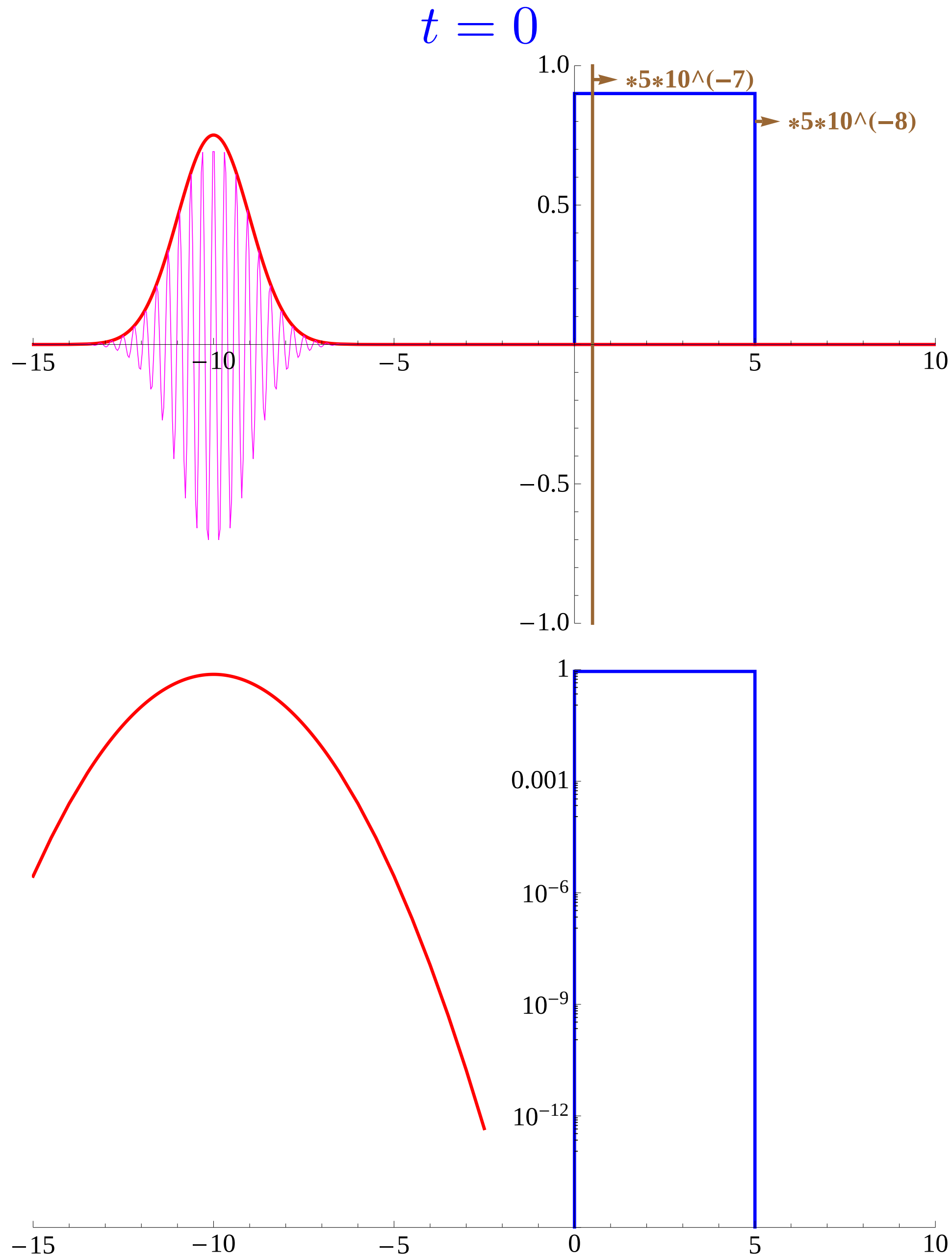
C: "Fast" wave packet, thick barrier

Parameters: $k_0 = 20 \gg \sigma_k$,
$L = 5 > \sigma_x, \gg \pi/k_0$, $\sigma_k = 1/\sqrt{2} \approx 0.7$,
$x_0 = -10$, $2m = 1$, $V = 25^2$

Momentum distribution $|A(k)|$:

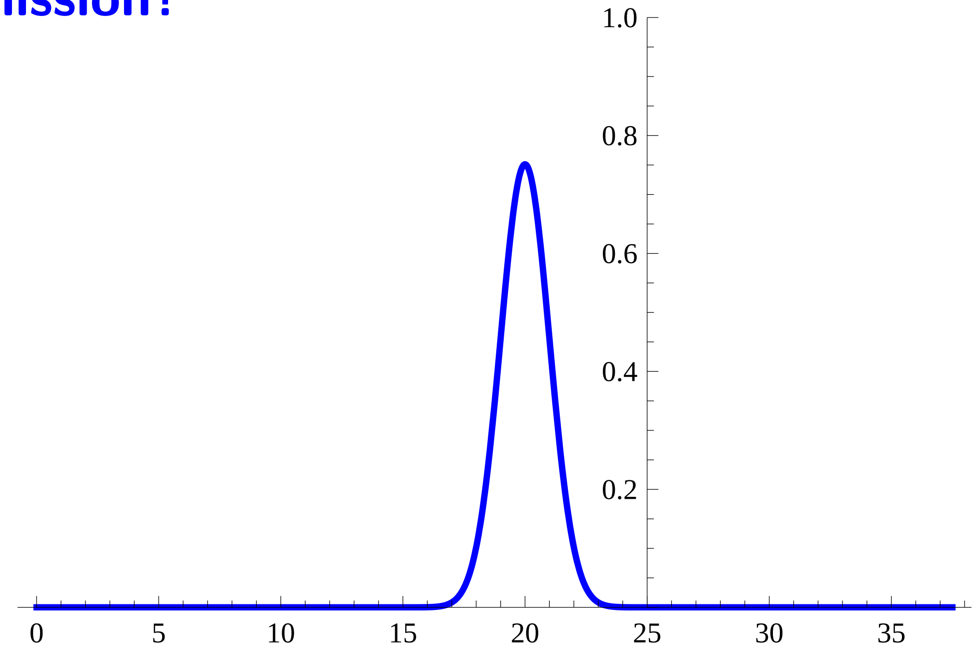


Right plots: barrier, $|\psi(t,x)|$, $\mathrm{Re}\,\psi(t,x)$;
top: to scale by $5{\cdot}10^{-7}$ for $0.5 < x < L$
and by $5{\cdot}10^{-8}$ for $x > L$;

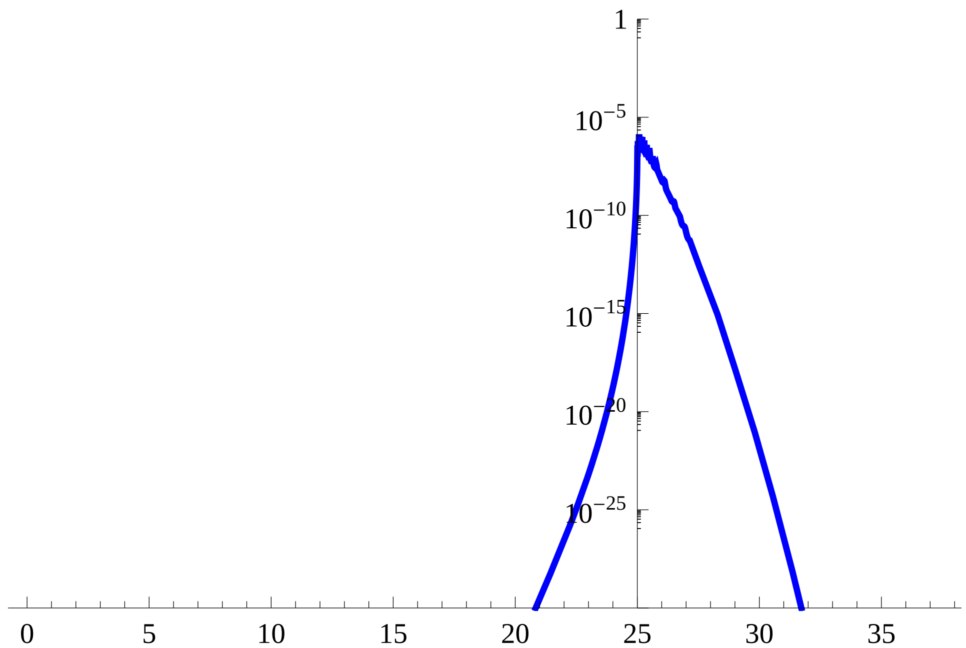


C: "Fast" wave packet, thick barrier — Which momenta contribute to the transmission?

Momentum distribution of incoming wave packet, i.e. part of $\tilde{\psi}(k;t,x) \propto e^{ikx}$ at $x < 0$: $|A(k)|$



Momentum distribution of transmitted wave packet, i.e. $\tilde{\psi}(k;t,x)$ at $x > L$: $|A(k)\,\tilde{\psi}(k;t,L)|$ (logarithmic scale)

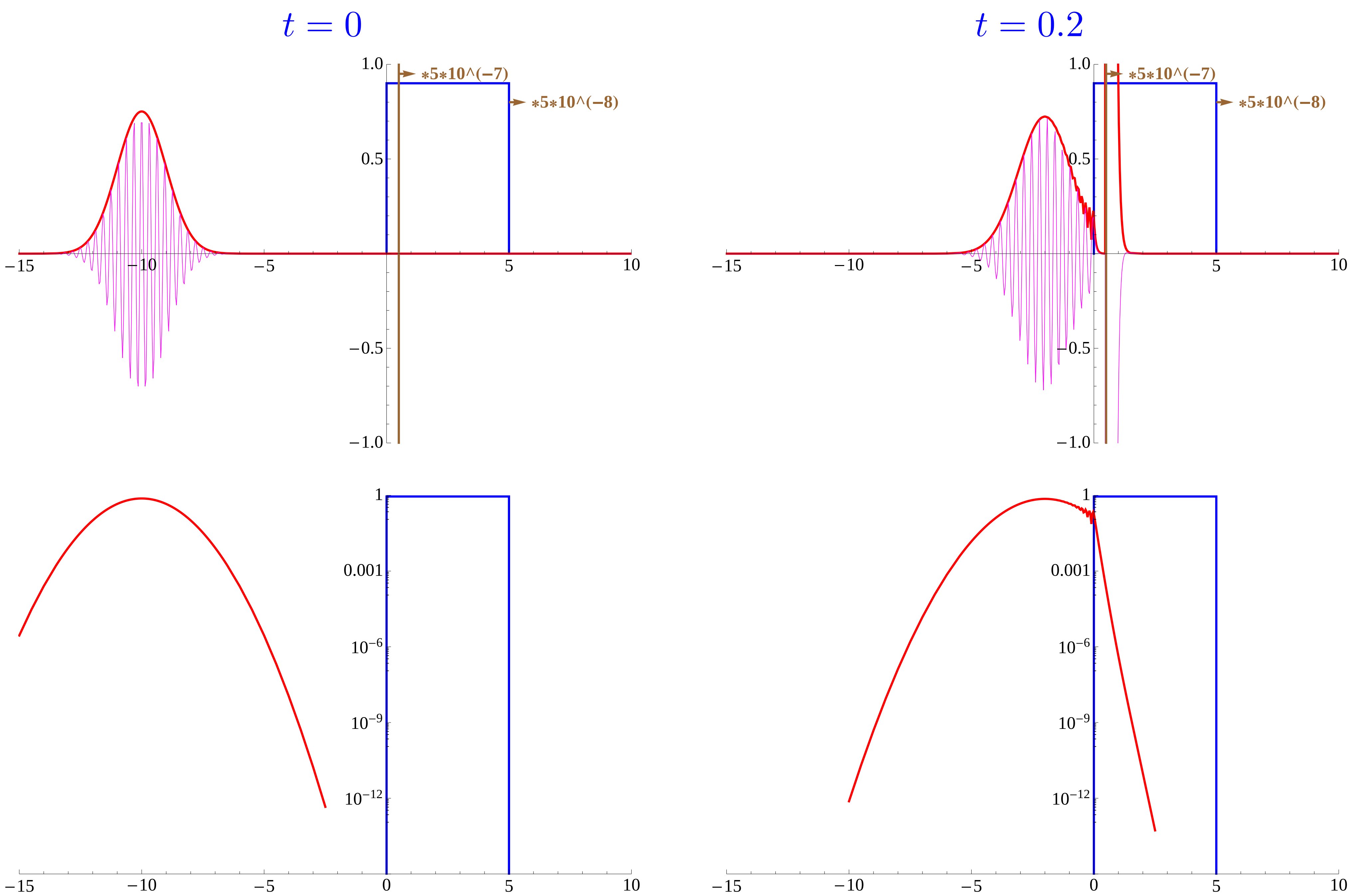


$\Rightarrow$ like in case B:

transmission dominated by high momenta $k \gtrsim \sqrt{V}$

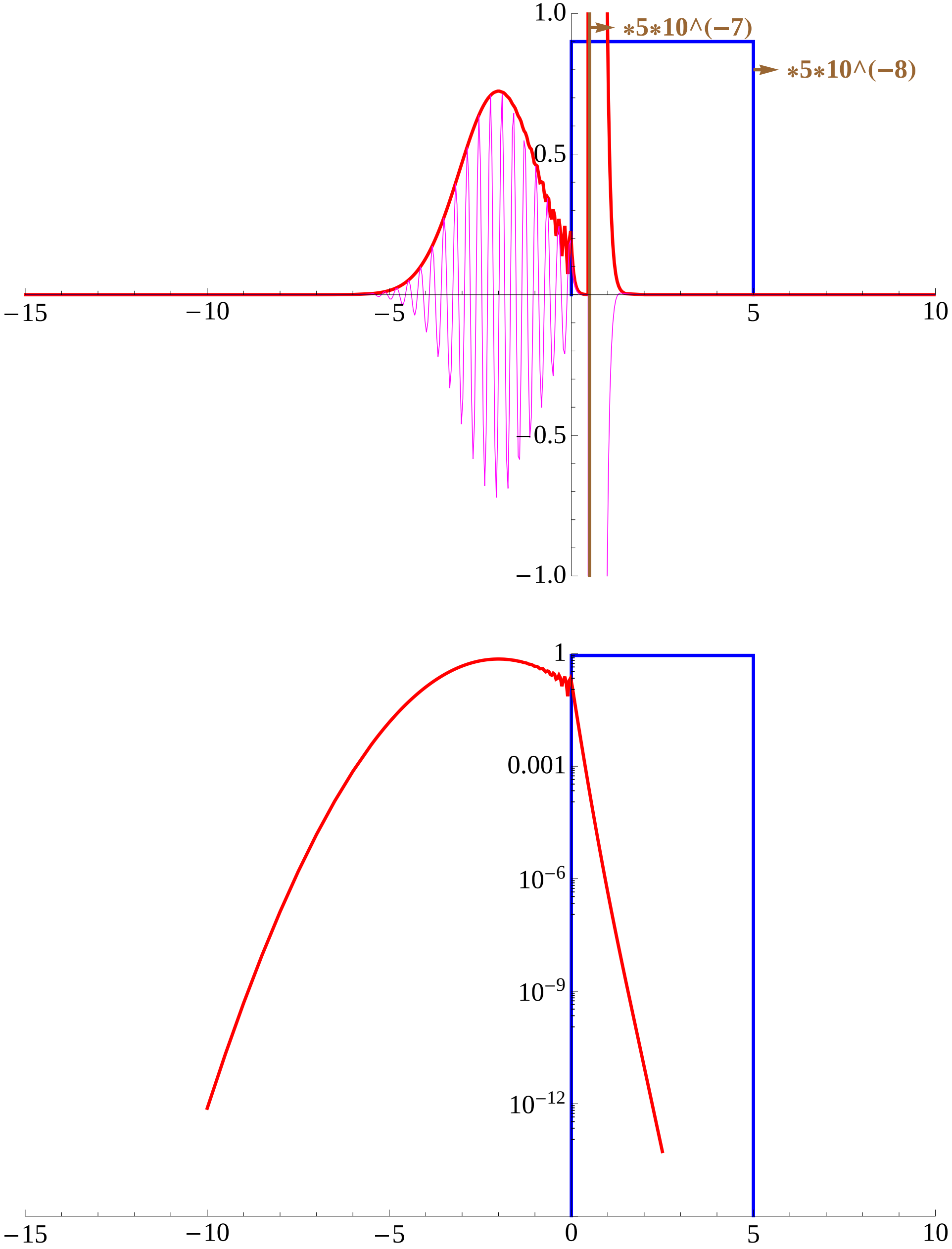
$\Rightarrow$ classically allowed transmission

C: "Fast" wave packet, thick barrier

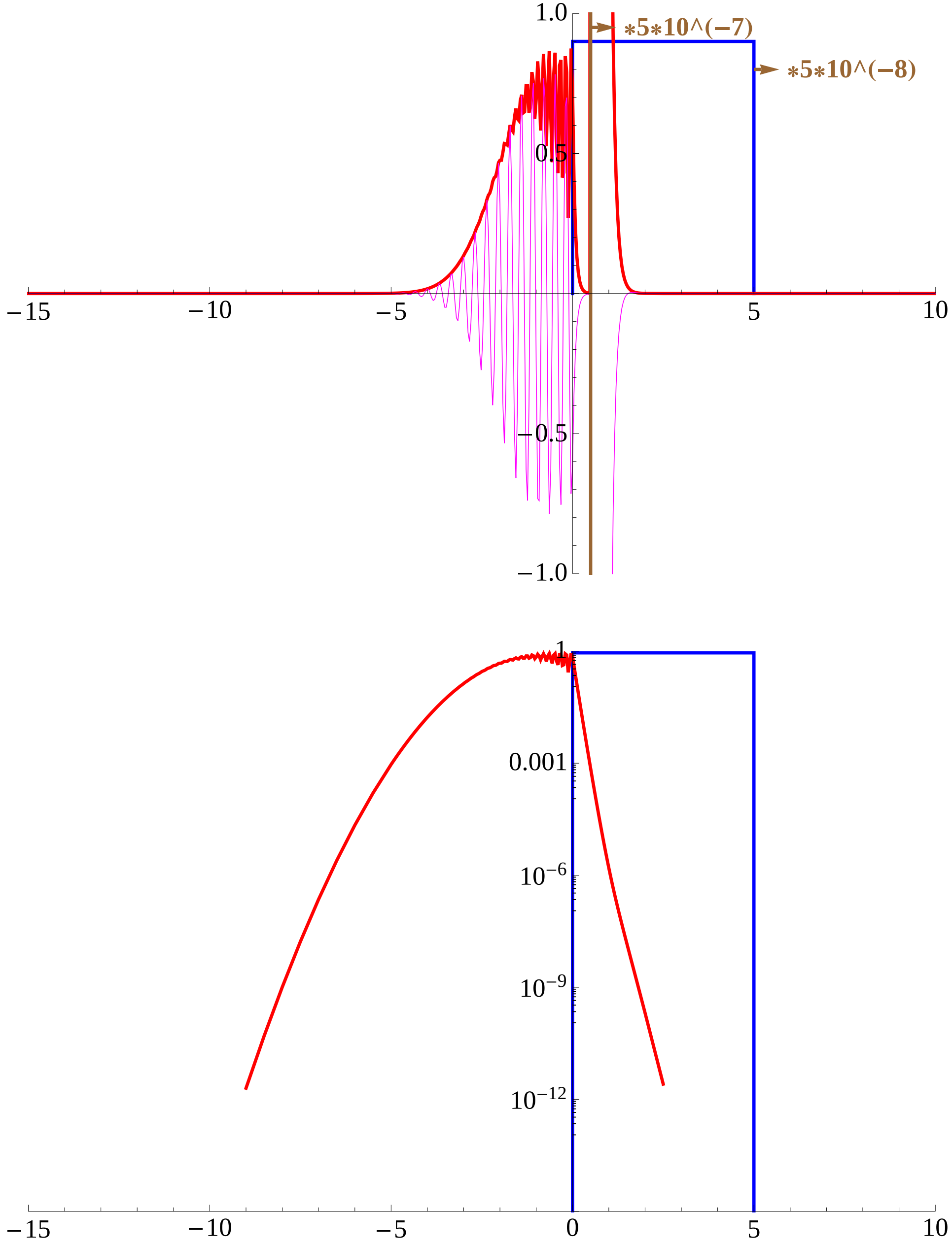


C: “Fast” wave packet, thick barrier

$t = 0.2$

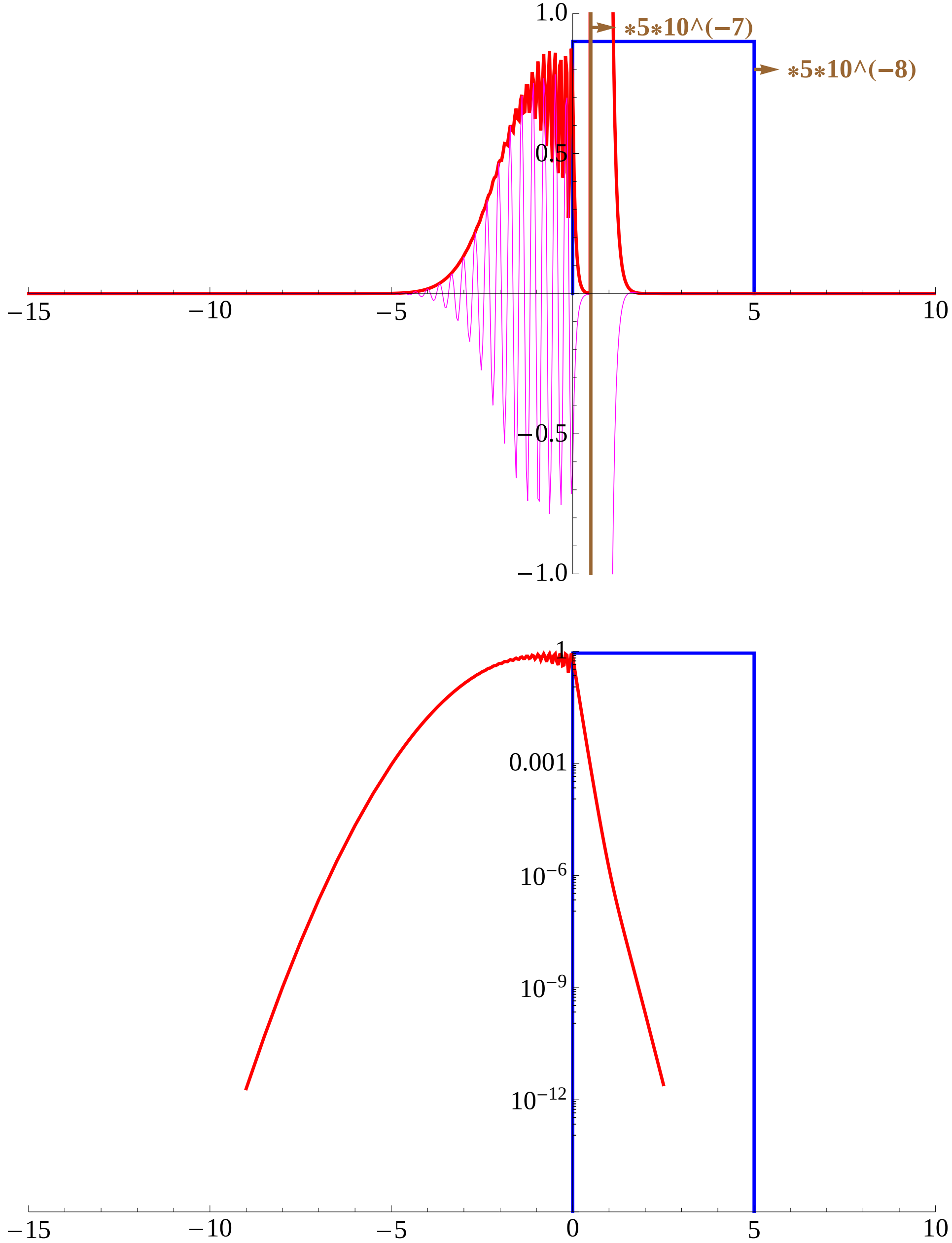


$t = 0.225$

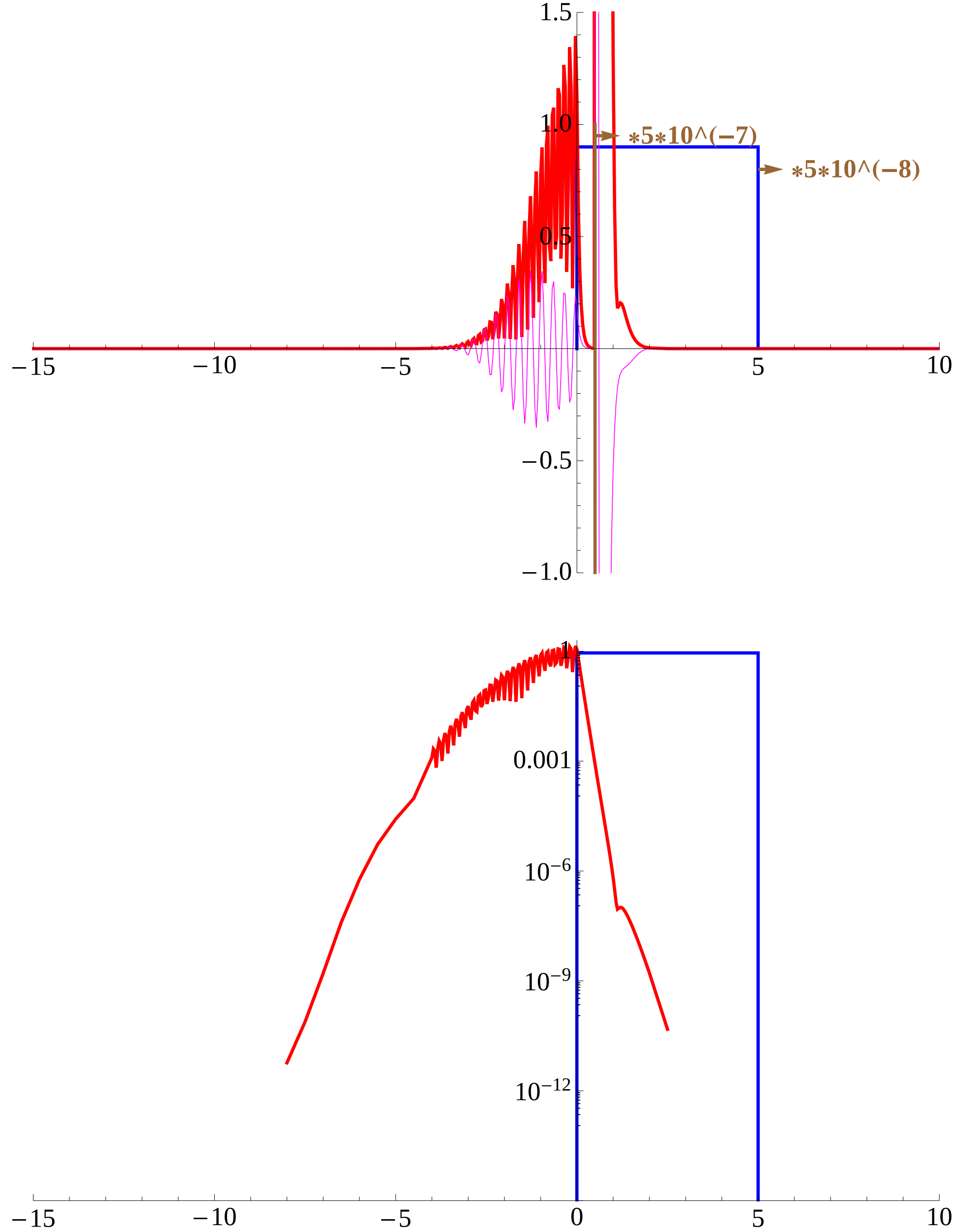


C: "Fast" wave packet, thick barrier

$t = 0.225$

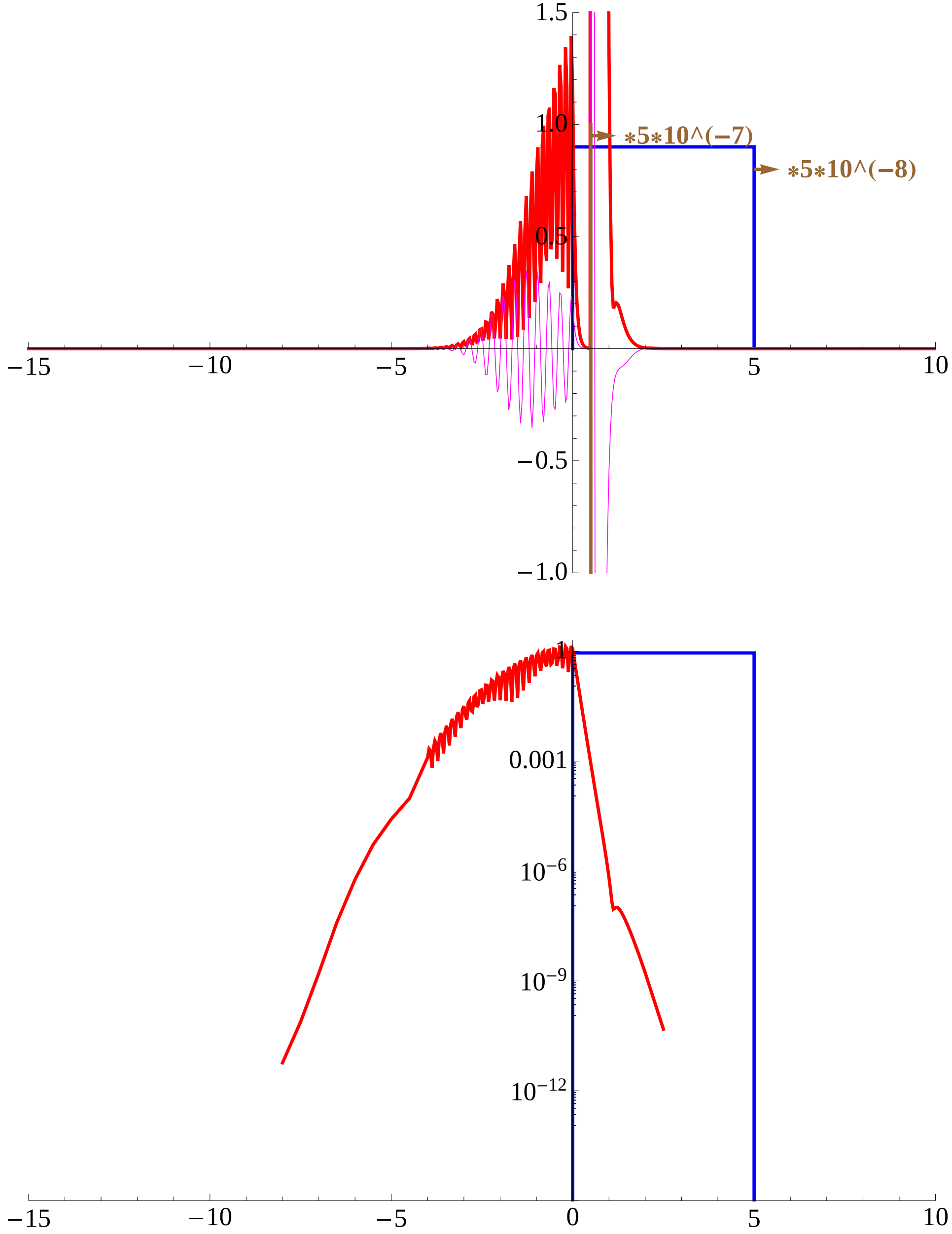


$t = 0.25$

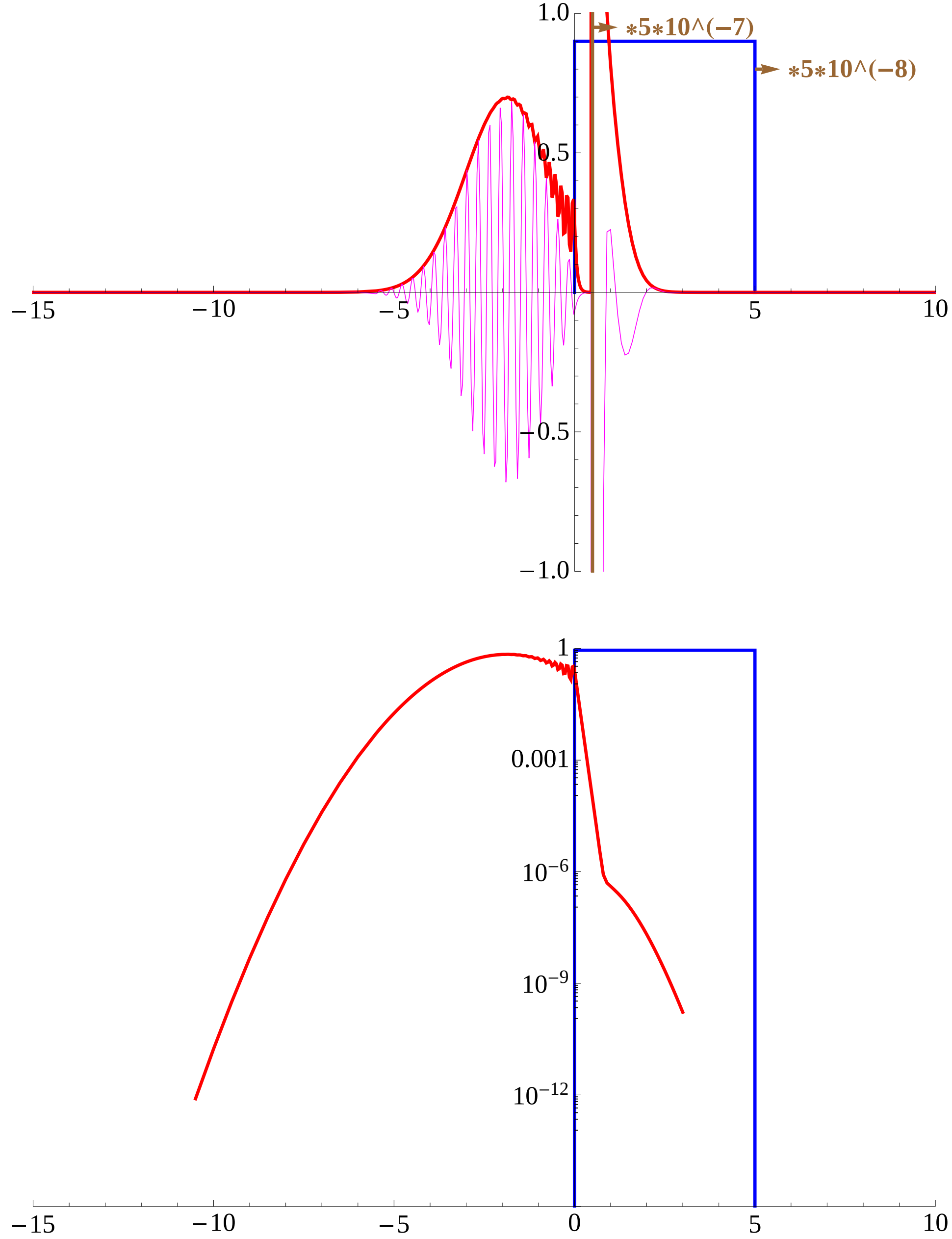


C: “Fast” wave packet, thick barrier

$t = 0.25$

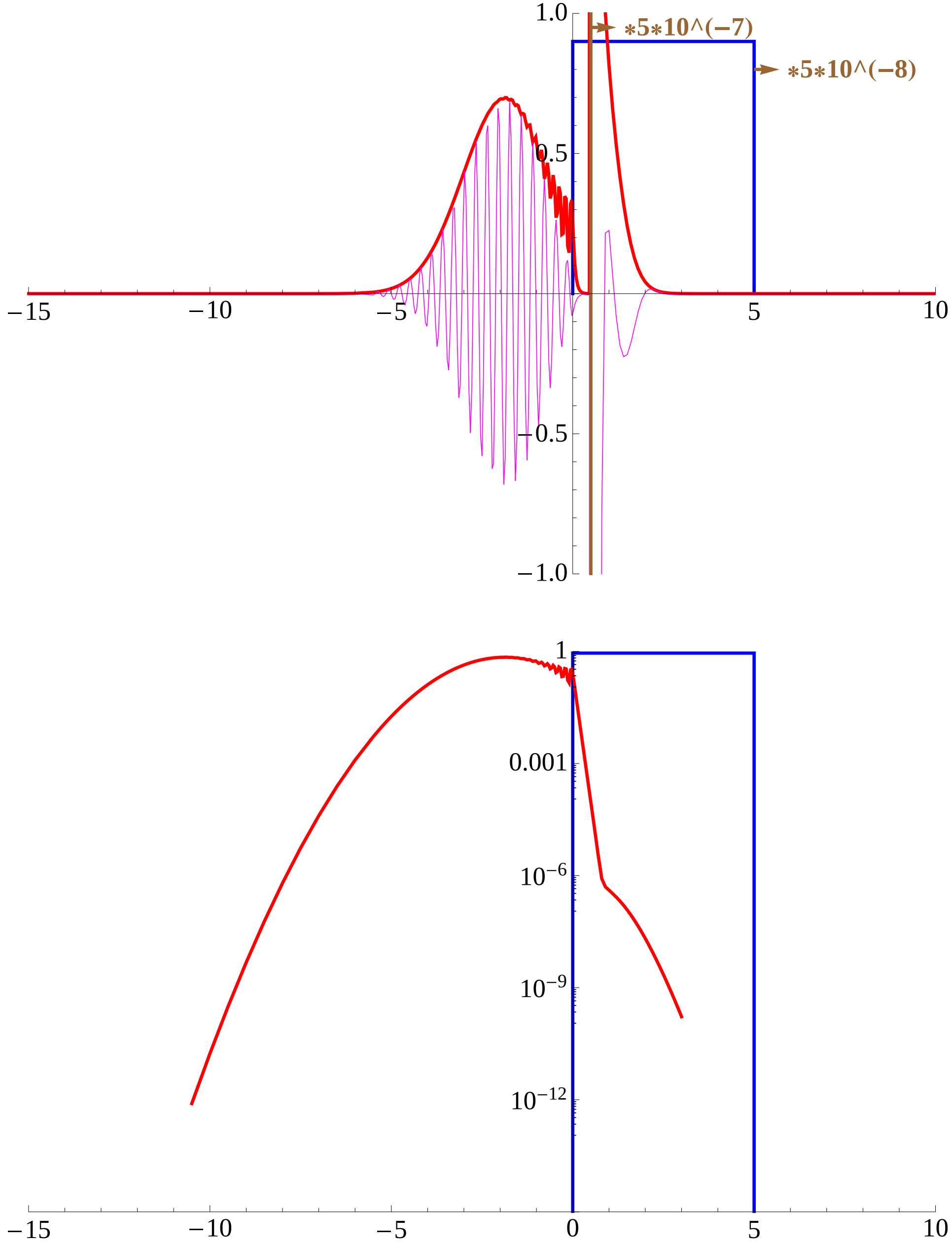


$t = 0.3$

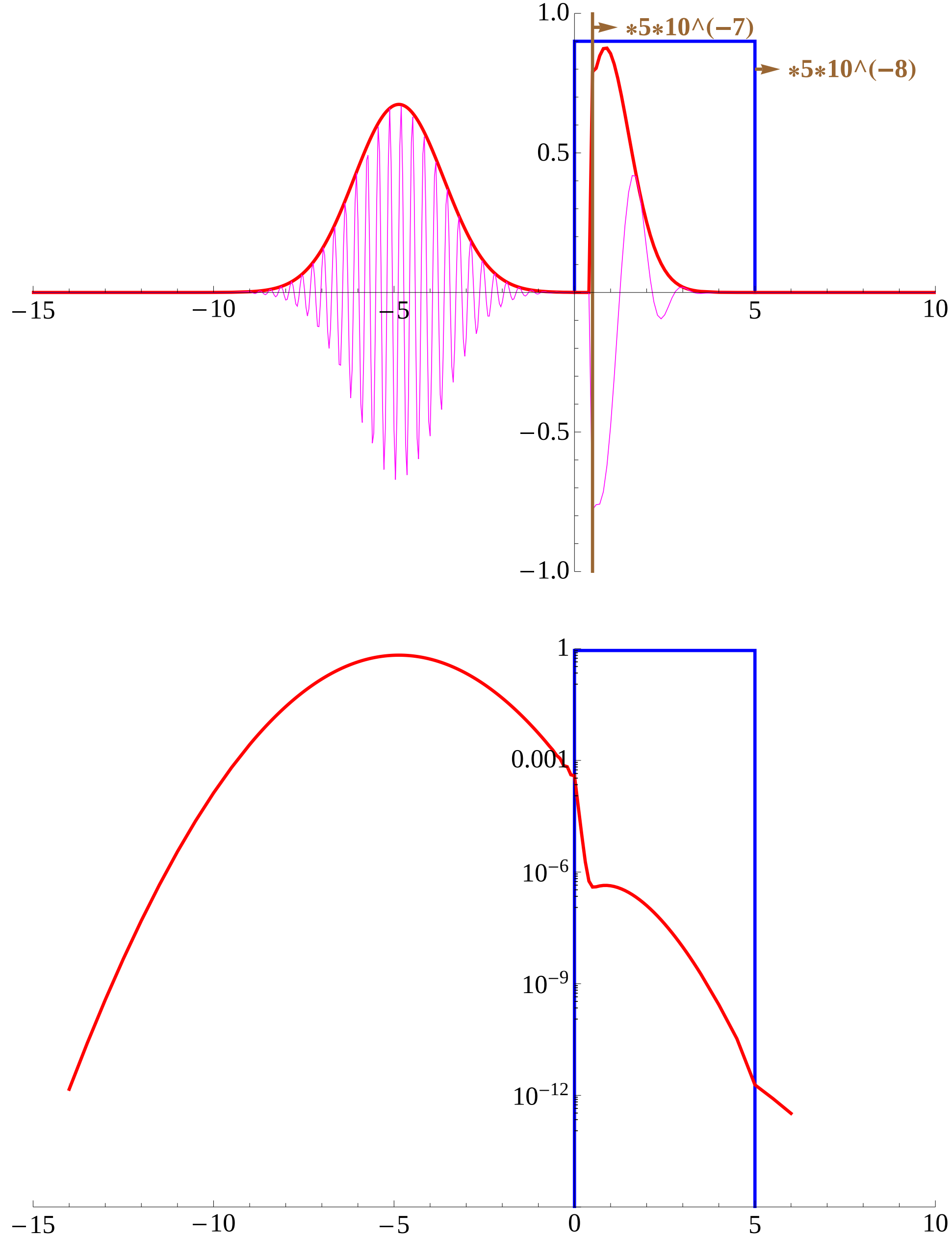


C: "Fast" wave packet, thick barrier

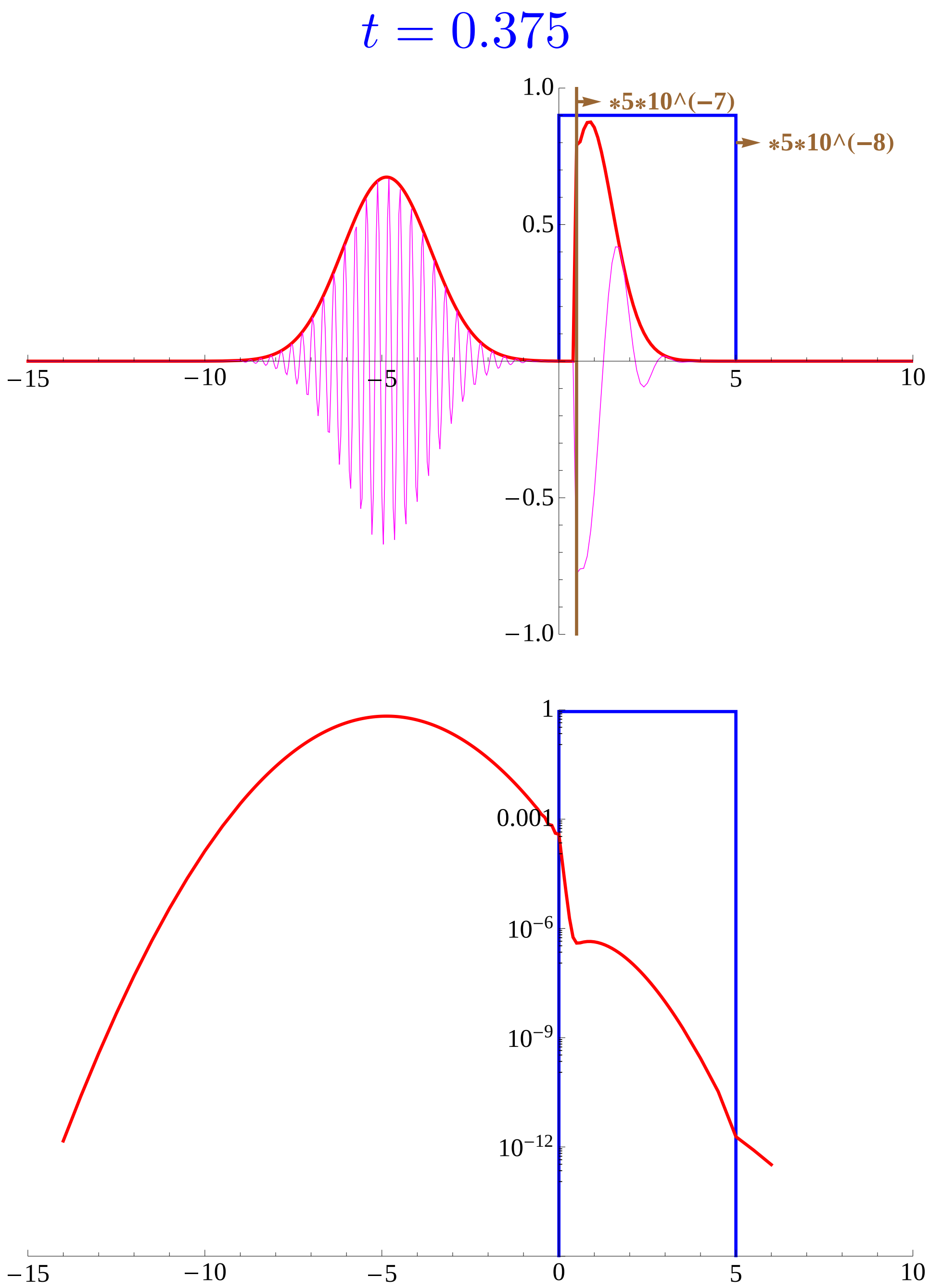
$t = 0.3$

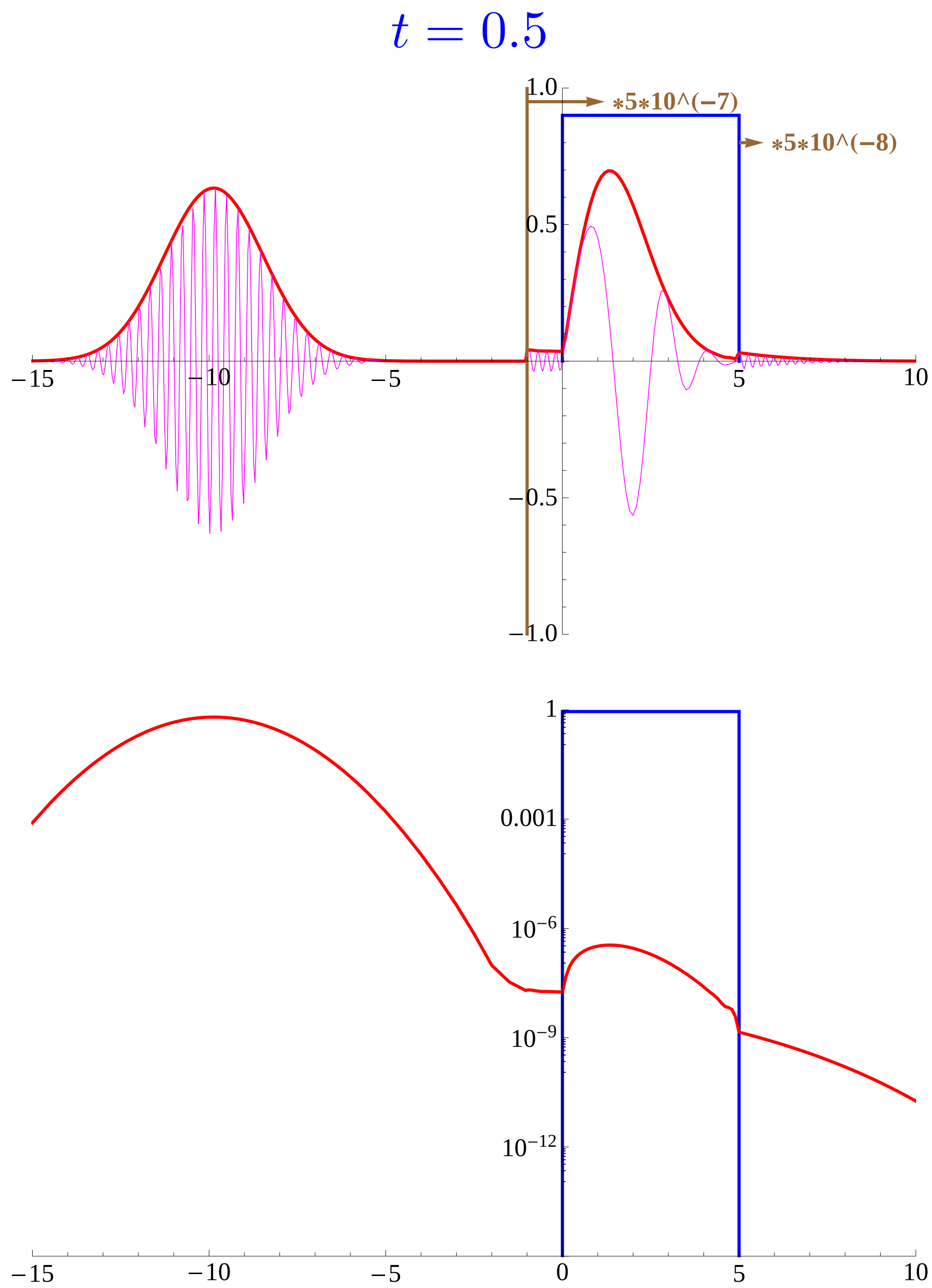


$t = 0.375$

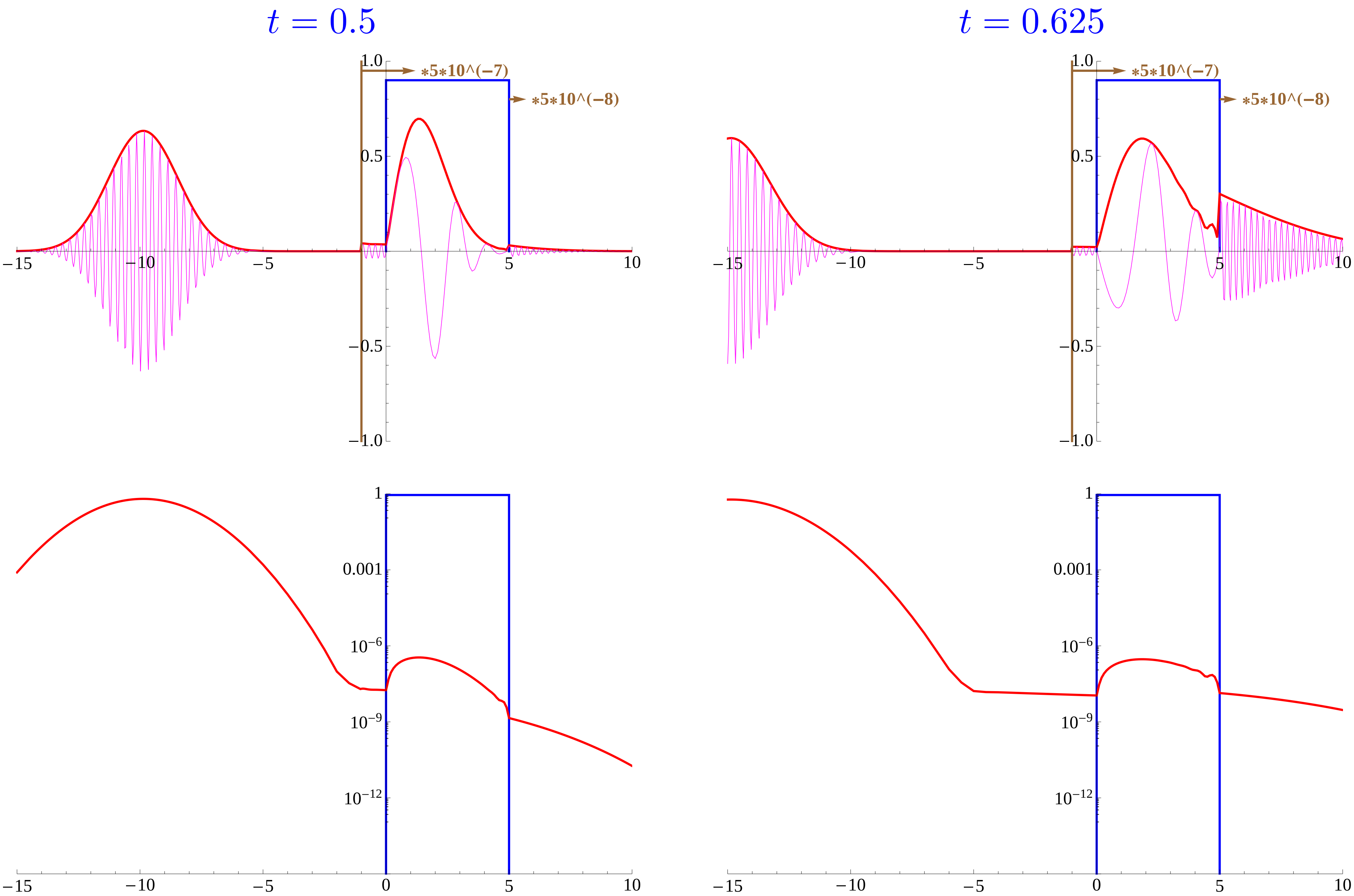


C: "Fast" wave packet, thick barrier



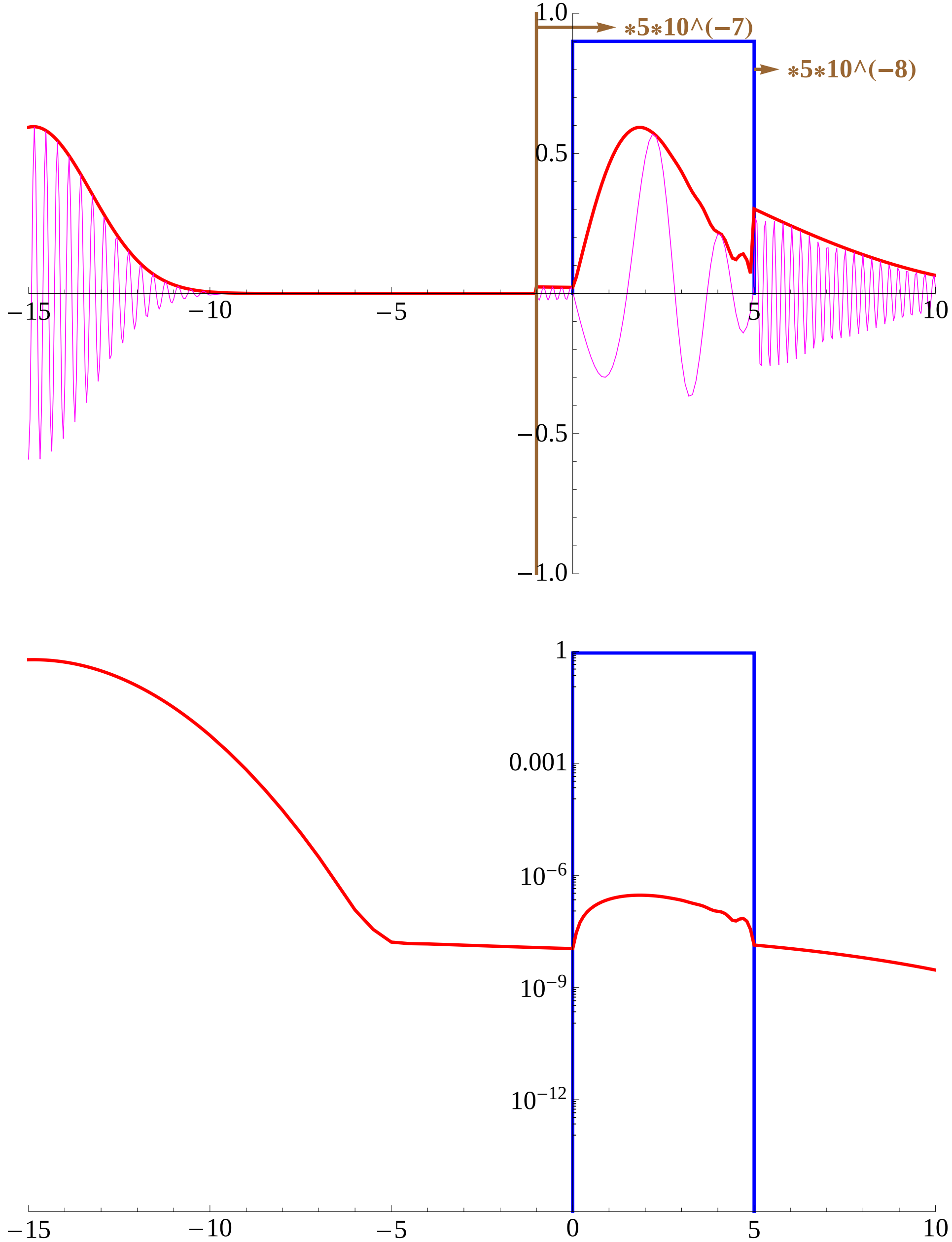


C: “Fast” wave packet, thick barrier

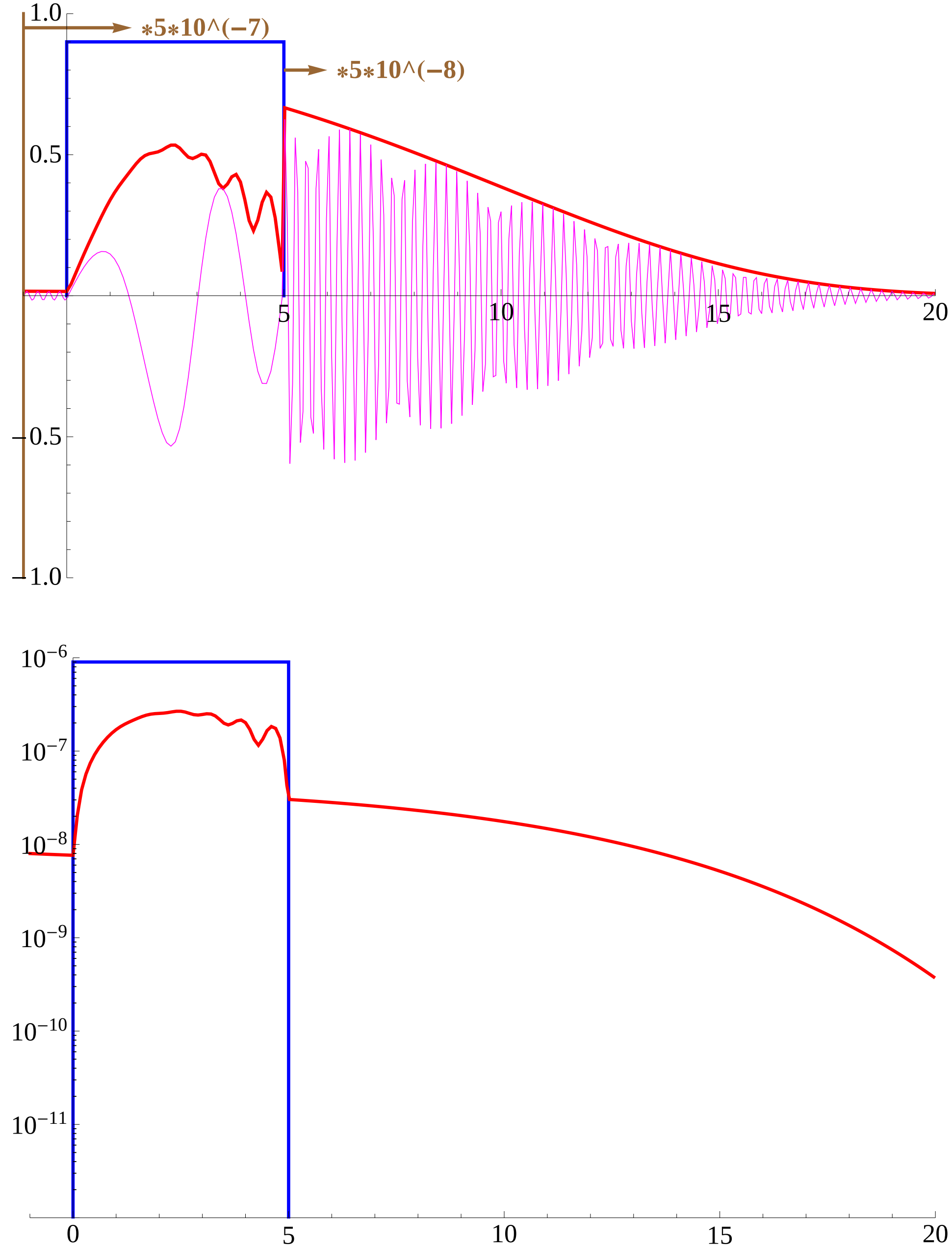


C: “Fast” wave packet, thick barrier

$t = 0.625$

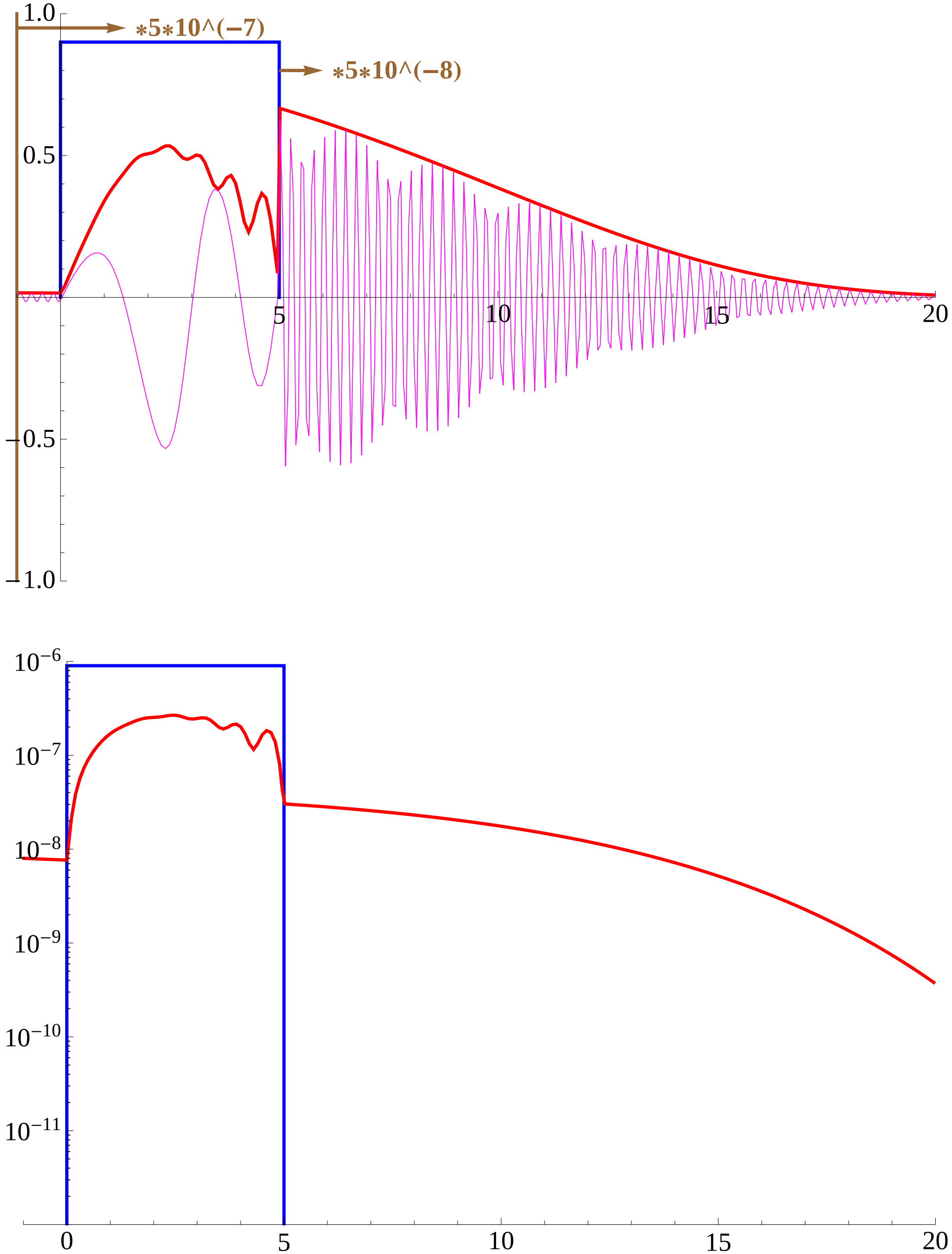


$t = 0.75$

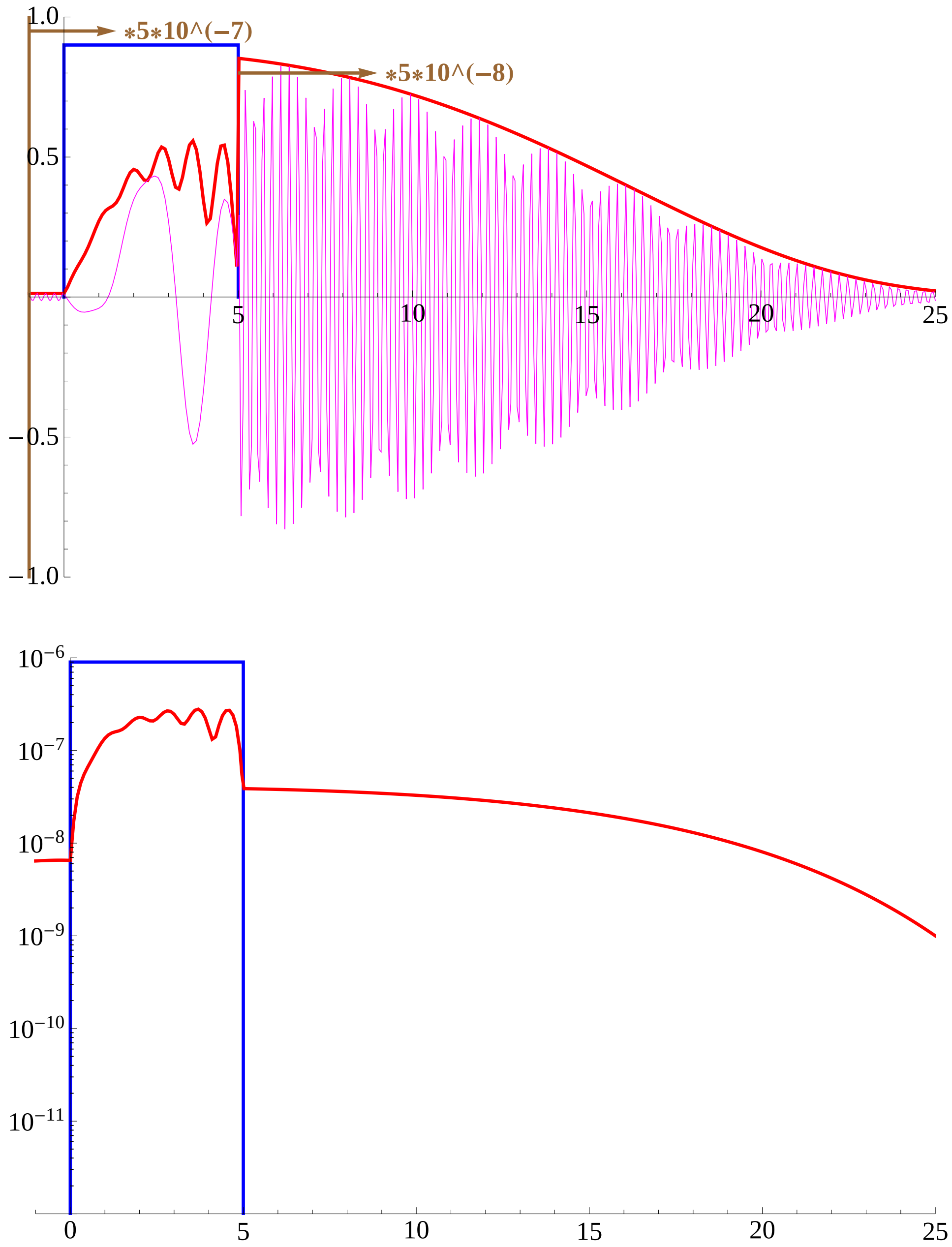


C: “Fast” wave packet, thick barrier

$t = 0.75$

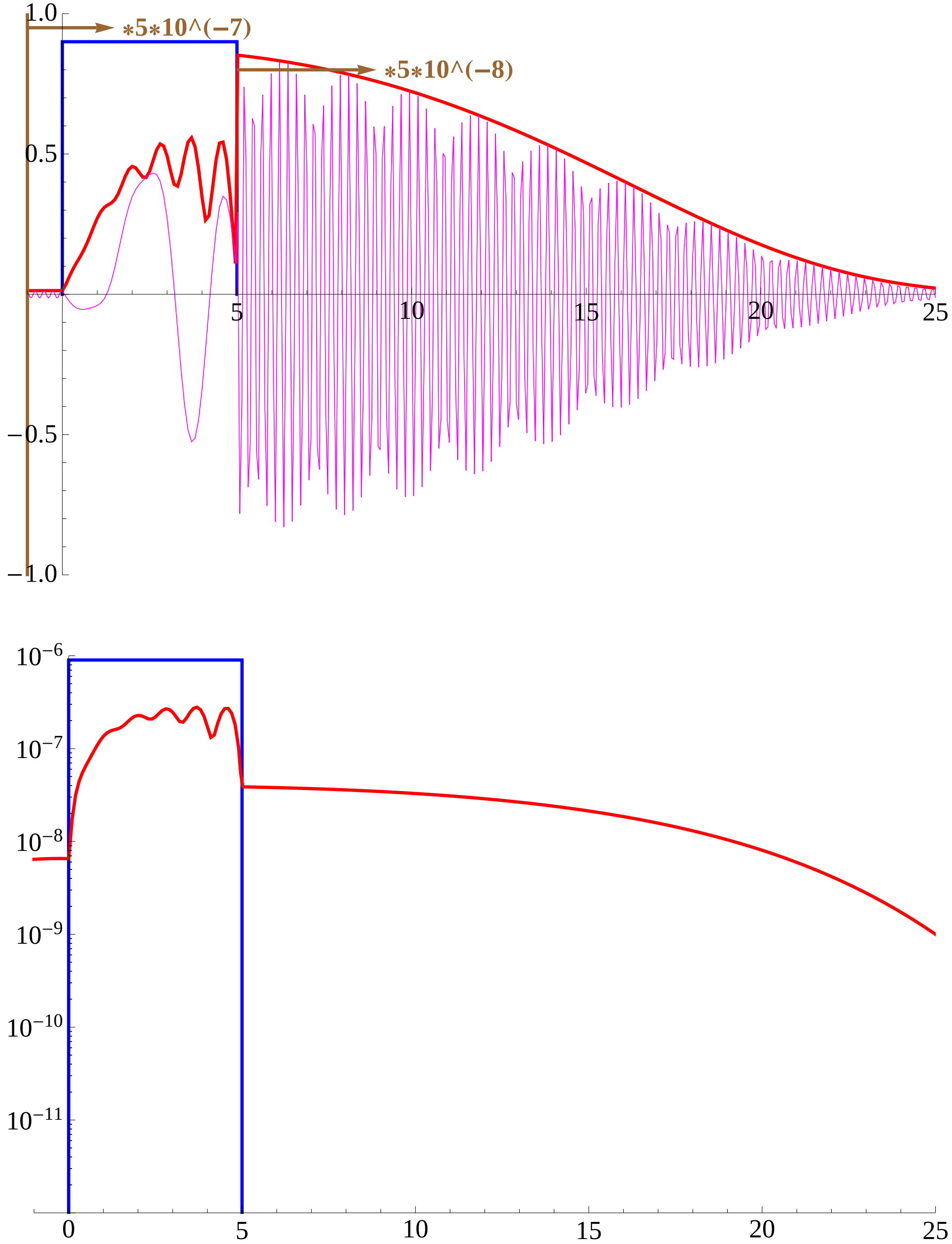


$t = 0.875$

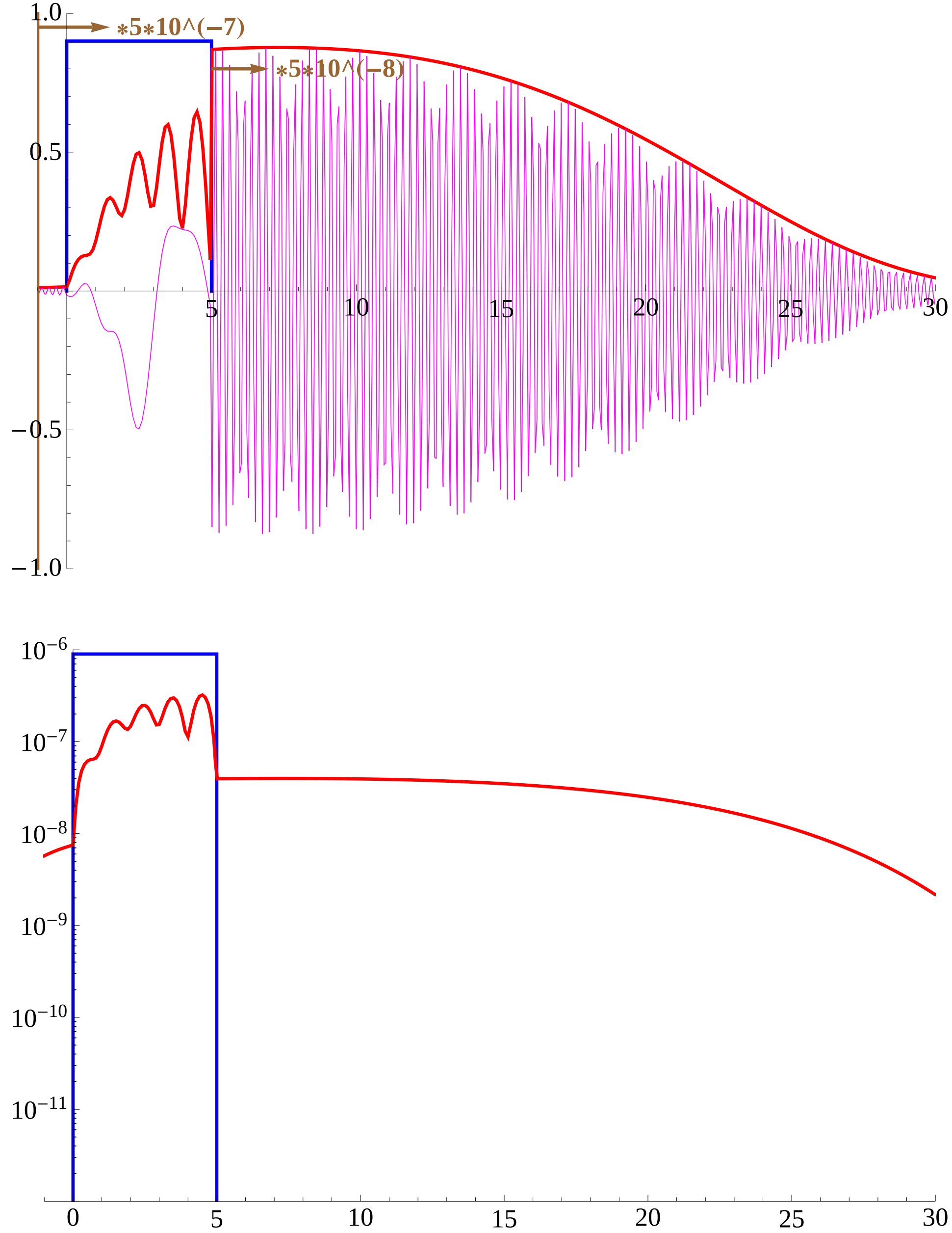


C: “Fast” wave packet, thick barrier

$t = 0.875$

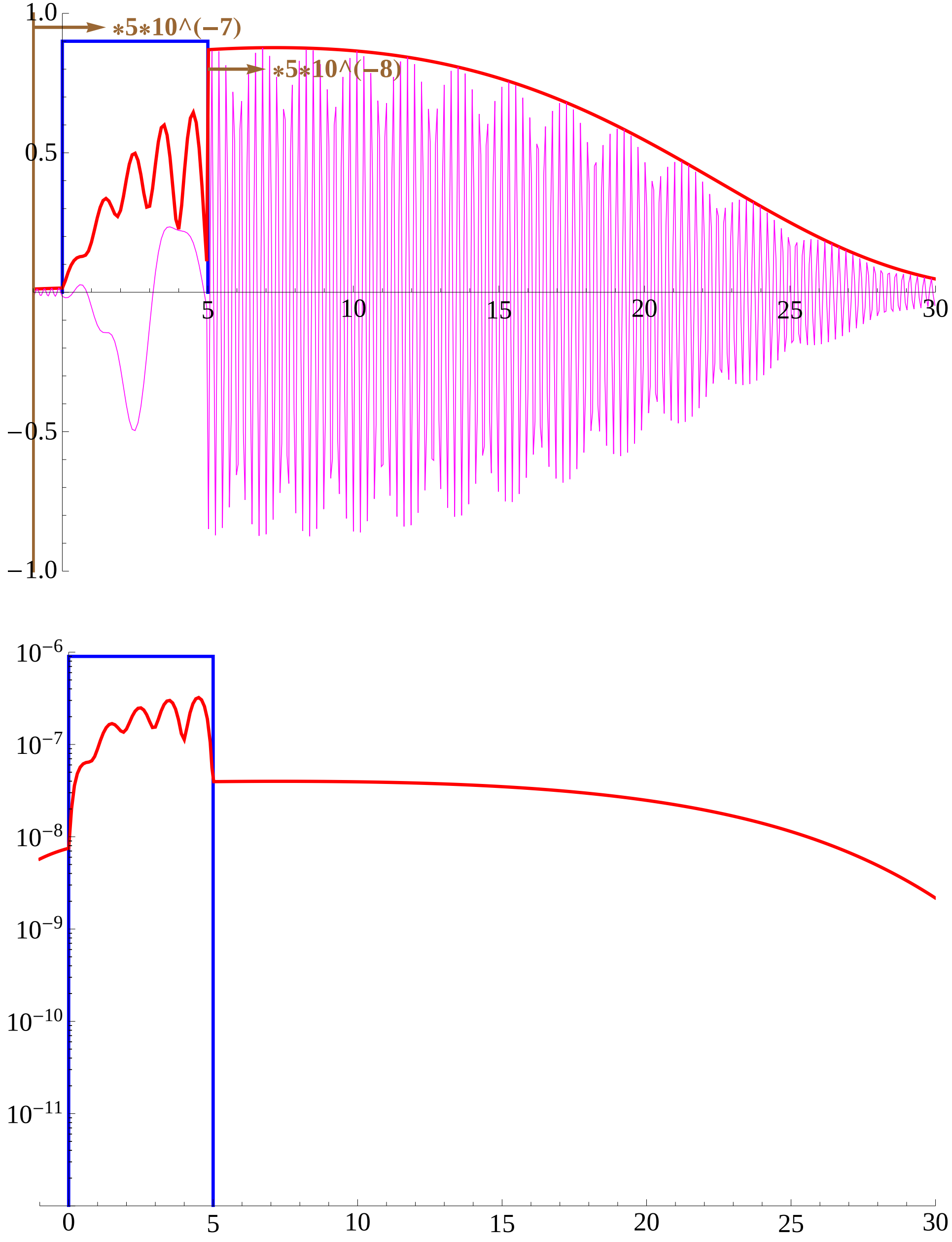


$t = 1$

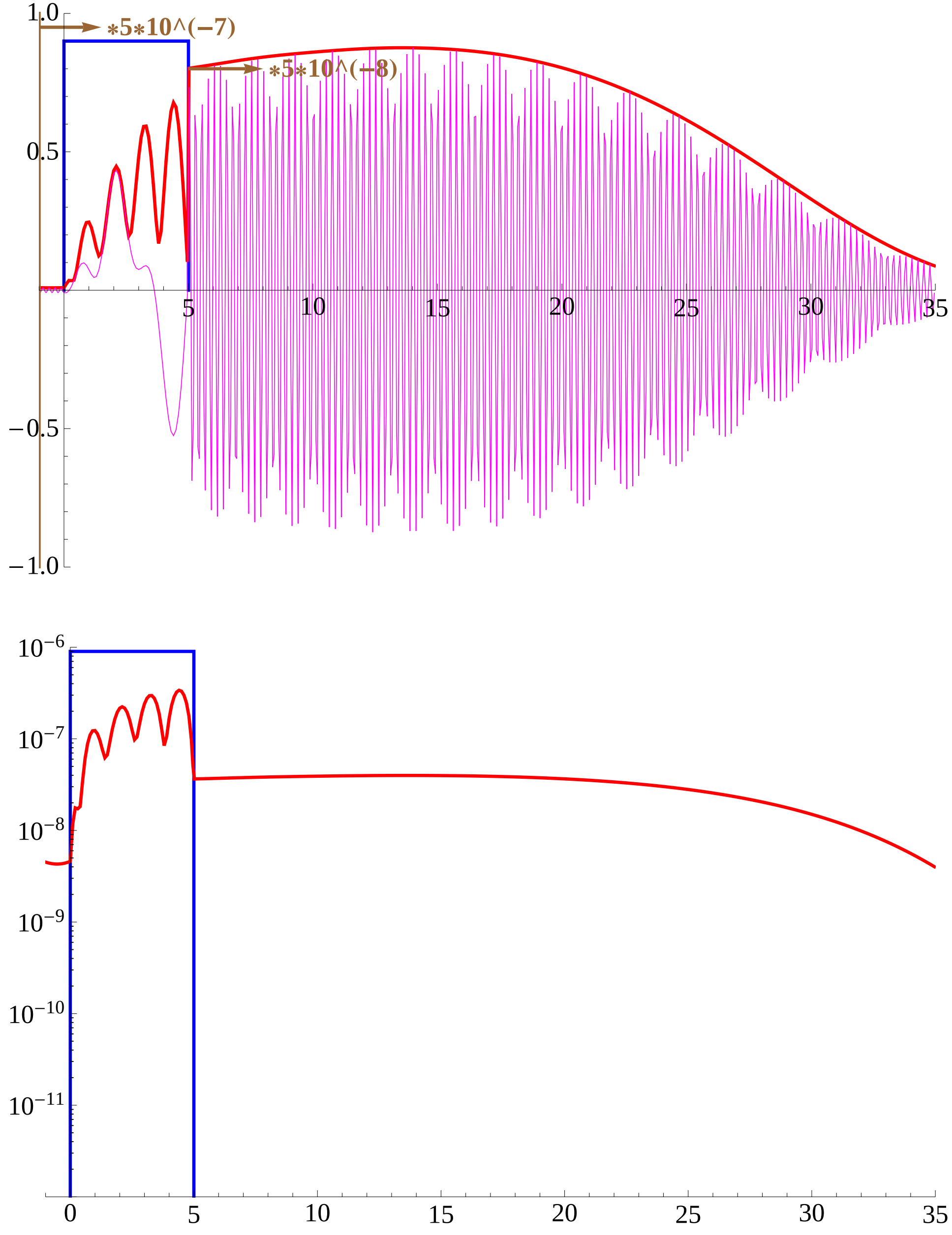


C: “Fast” wave packet, thick barrier

$t = 1$

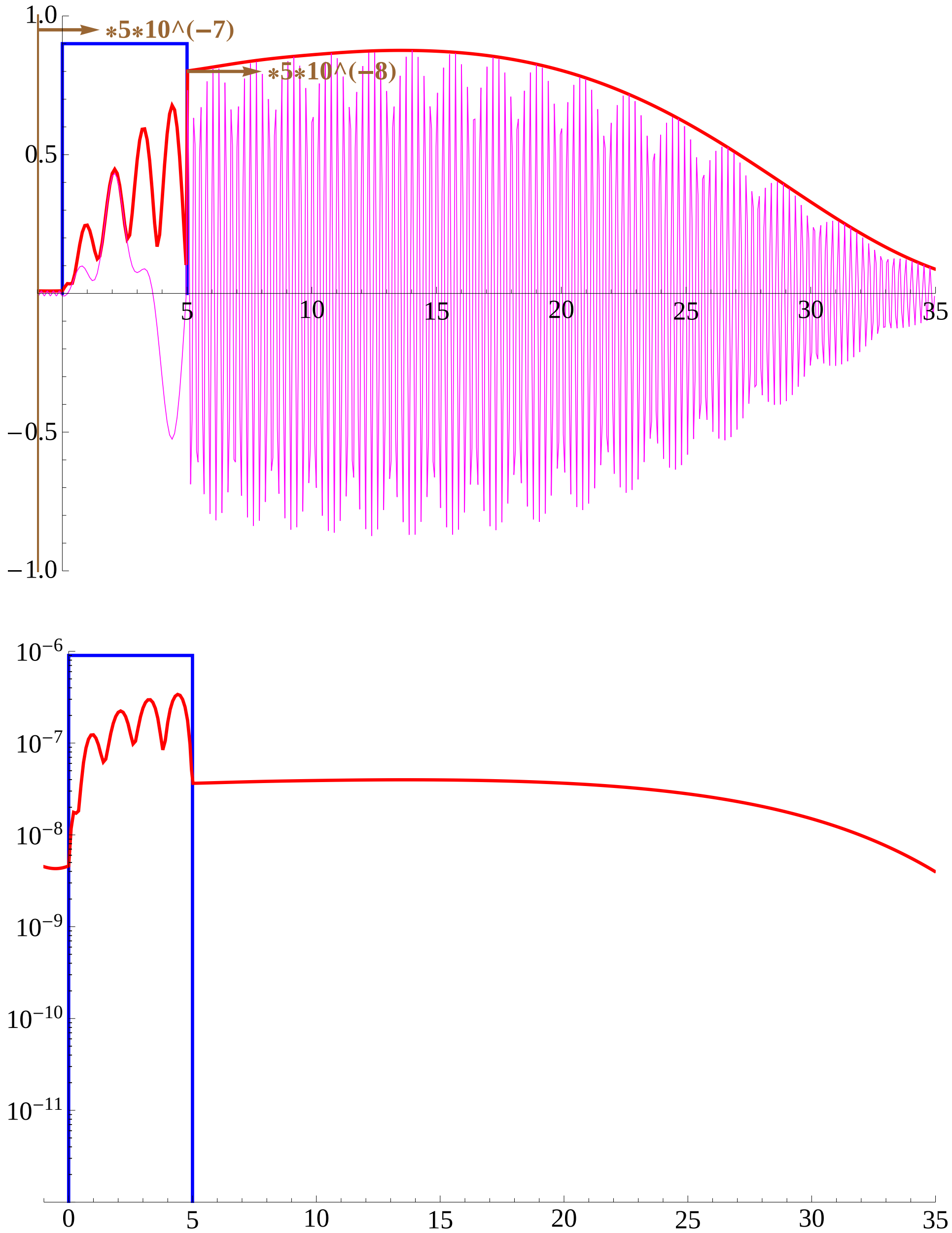


$t = 1.125$

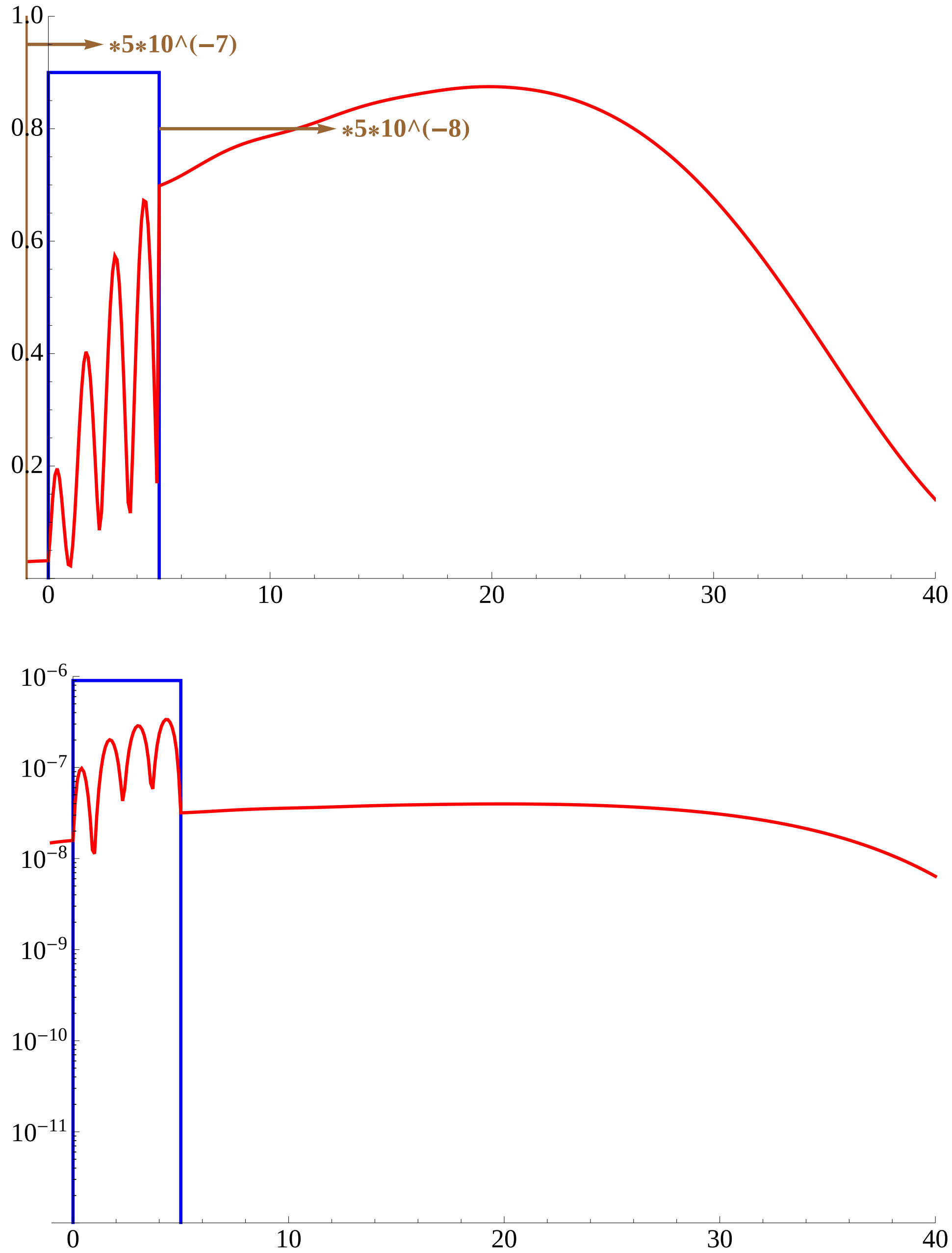


C: "Fast" wave packet, thick barrier

$t = 1.125$

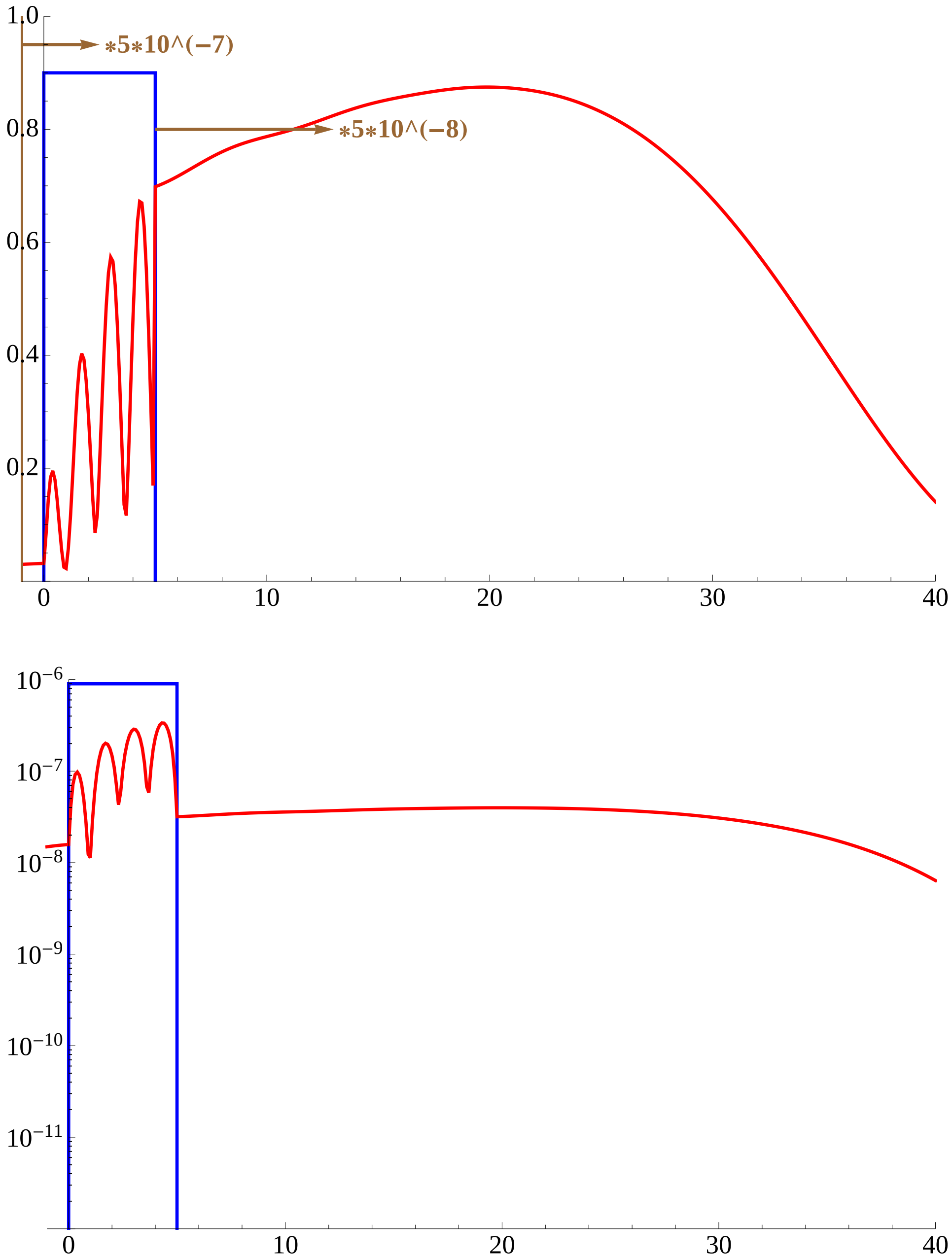


$t = 1.25$

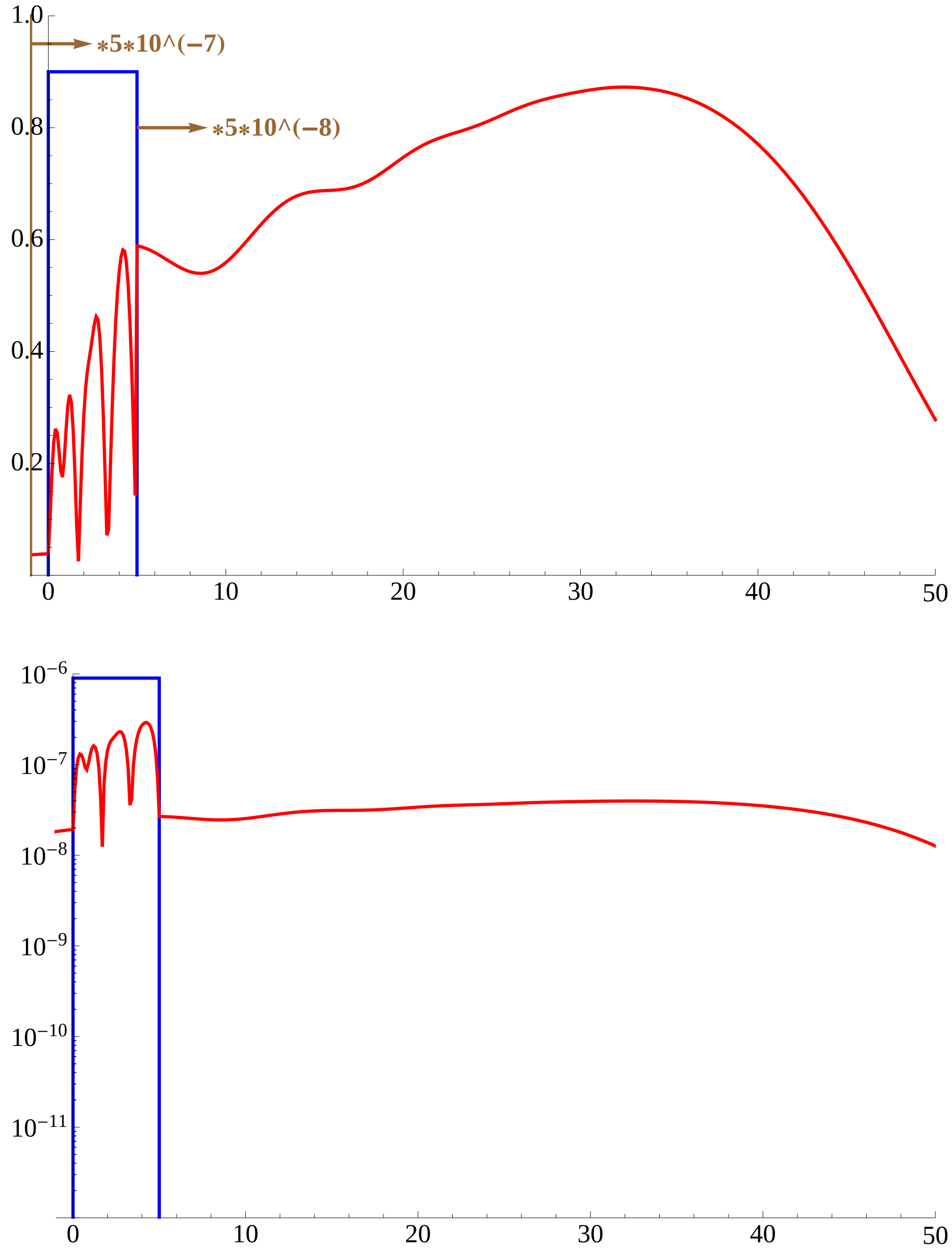


C: "Fast" wave packet, thick barrier

$t = 1.25$

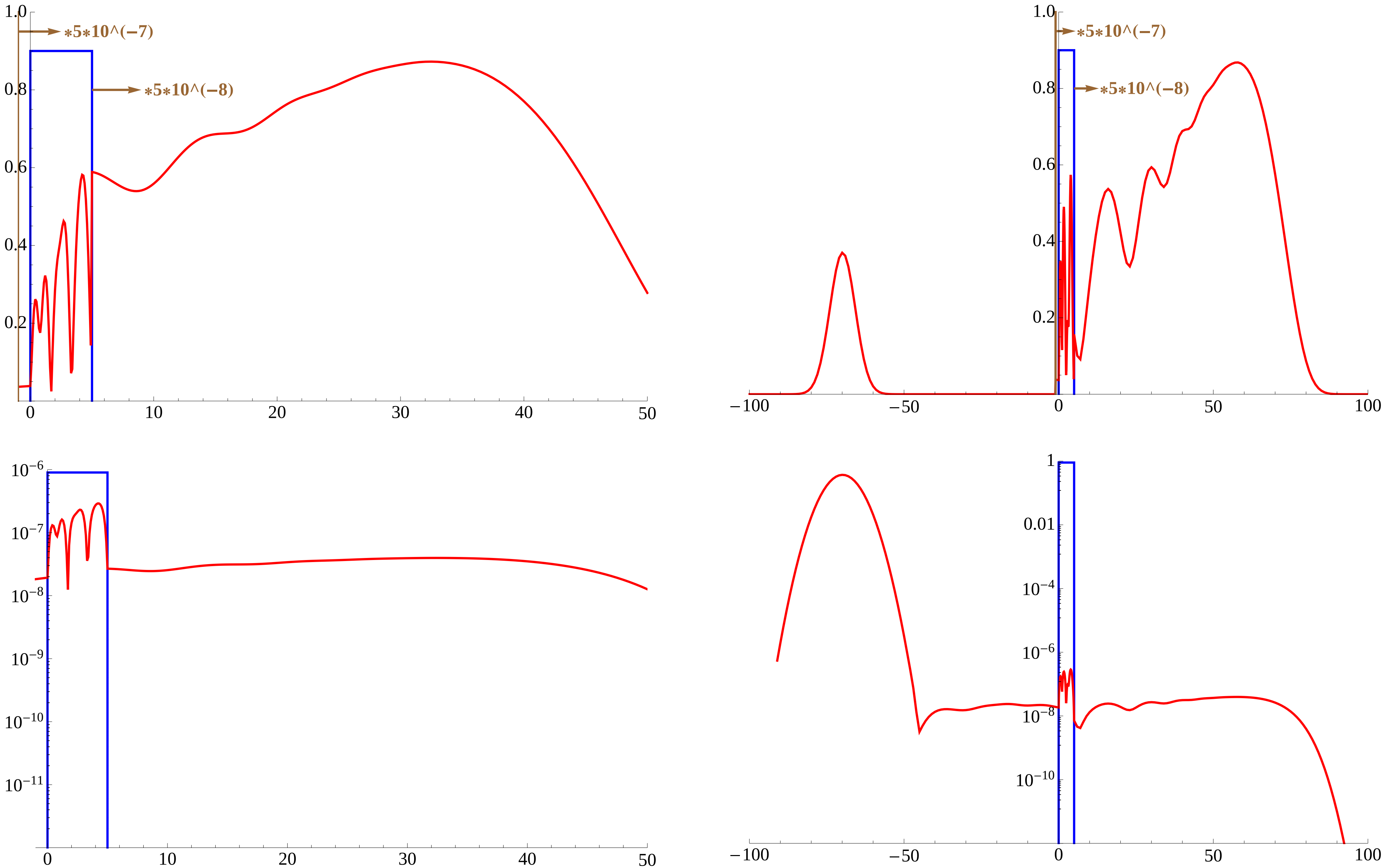


$t = 1.5$



C: “Fast” wave packet, thick barrier

$t = 1.5$ $t = 2$



C: "Fast" wave packet, thick barrier — Conclusion

- "Fast" wave packet: σ_k/k_0 smaller, (almost) no low momenta
  $\hookrightarrow$ wave packet stays more compact $\Rightarrow$ better time resolution
- Thick barrier: like in case B – strong exponential damping ($\sim 10^{-30}$ at k_0)
  $\hookrightarrow$ dominated by classically allowed transmission of high momenta ($\sim 10^{-7}$).
- Incoming and reflected wave packet: like in cases A&B – wave length and velocity of maximum correspond to $k_0 = 20$ and to a reflection at $x = 0$.
- In the tunnel: a wave packet with moving maximum and large wave length appears, extends, is reflected from end of tunnel, develops fringes, becomes a standing wave
- Transmitted wave packet: wave length and velocity of maximum
  $\rightsquigarrow k \approx 25 = \sqrt{V} > k_0$
- Packet maximum enters tunnel at $t = 0.25$ and exits at $t = 0.95$
  $\Rightarrow \Delta t_{\text{tunnel}} \approx 0.7 > 0$ ($v_{\text{tunnel}} = L/\Delta t_{\text{tunnel}} \approx 7.1 \rightsquigarrow k_{\text{tunnel}} \approx 3.6 \ll k_0$)
- Like in case B: transmitted wave packet develops tail of lower maxima.