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Yukawa KPZ

Anharmonic Chains and Multi-Component KPZ Equations

Herbert Spohn

TU Munich

joint work with

P. Ferrari (Bonn)
C. Mendl (TUM)
T. Sasamoto (Tokyo)

1D KPZ equation

$$\partial_t h = \frac{1}{2}(\partial_x h)^2 + \frac{1}{2}\partial_x^2 h + \xi$$

$\Rightarrow$

multi-component KPZ

ξ space-time white noise

component index α

$$\partial_t h_\alpha = -c_\alpha \partial_x h_\alpha + \langle \partial_x \vec{h}, G^\alpha \partial_x \vec{h} \rangle + \partial_x^2 (D\vec{h})_\alpha + (B\vec{\xi})_\alpha \quad , \ \alpha = 1, \dots, n$$

$2D = BB^T$

Ertaş, Kardar 2003 all $c_\alpha = 0$, mostly $n = 2$

HERE // c_α are distinct // mostly $n = 3$

$\vec{c} = (-c, 0, c)$

- Why should one care?

anharmonic chains

1 D fluids, also quantum

multi-component stochastic lattice gases

⋮

- What can be analysed?

Contents

1. theoretical results
2. anharmonic chains
3. MD simulations

hard point collisions

FPU chains

1. multi-component KPZ

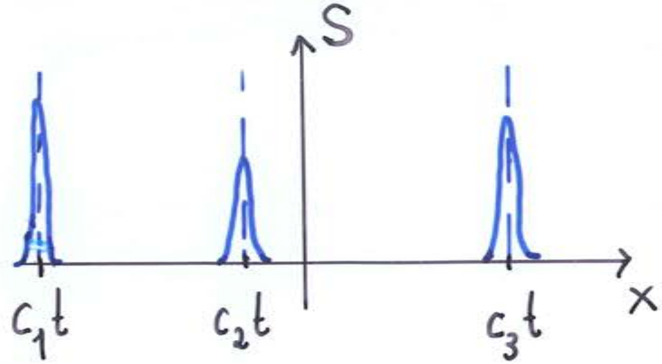
Gaussian theory $\qquad \partial_t h_\alpha = -c_\alpha \partial_x h_\alpha + \partial_x^2 (D\vec{h})_\alpha + (B\vec{\xi})_\alpha$

slope $\qquad \phi_\alpha = \partial_x h_\alpha$

stationary measure $\qquad \langle \phi_\alpha(x) \rangle = 0, \quad \langle \phi_\alpha(x)\, \phi_{\alpha'}(x') \rangle = \delta_{\alpha\alpha'}\, \delta(x-x')$

- covariance

  $$S_{\alpha\beta}(x,t) = \langle \phi_\alpha(x,t)\, \phi_\beta(0,0) \rangle$$



- large x, t

  $\sqrt{t}$ broadening

  peaks decouple, shape function is Gaussian* nonlinear theory stationary

Decoupling Conjecture

If $G^{\alpha}_{\alpha\alpha} \neq 0$, then peak α is in the KPZ universality class

examples: $\langle \phi_\alpha(x,t)\, \phi_\alpha(0,0) \rangle$

broadening as $t^{2/3}$, KPZ scaling function, ...

some rigorous results

I) invariant measures

If $G^{\alpha}_{\beta\gamma} = G^{\alpha}_{\gamma\beta} = G^{\beta}_{\alpha\gamma}$, then Gaussian measure of linear theory is invariant

by definition

II lattice gases, Bethe ansatz, see Ferrari, Sasamoto, H.S. 2014

III harmonic chain, random collisions $(p_j, p_{j+1}) \Leftrightarrow (p_{j+1}, p_j)$

corresponds to

$$\partial_t \phi_\sigma + \partial_x(\sigma c \phi_\sigma - \partial_x \phi_\sigma + \xi_\sigma) = 0 \quad , \quad \sigma = \pm 1 \quad \text{independent}$$

$$\partial_t \phi_0 + \partial_x(\phi_1^2 - \phi_{-1}^2 - \partial_x \phi_\sigma + \xi_0) = 0 \quad \text{feed back}$$

RESULT: $\langle \phi_\sigma(x,t)\, \phi_\sigma(0,0) \rangle$ diffusive, $\sigma = \pm 1$

$$\langle \phi_0(x,t)\, \phi_0(0,0) \rangle \cong t^{-2/3} f_0(t^{-2/3} x)$$

!

Komorowski, Milton, Olla 2014

BUT $\hat{f}_0(k) = e^{-|k|^{3/2}}$

symmetric Levy $\frac{3}{2}$

III mode coupling theory   closed equation for S

$$\partial_t S_{\alpha\beta}(x,t) = \sum_{\alpha'=1}^{n} \Big\{ \left(-c_\alpha \delta_{\alpha\alpha'} \partial_x + D_{\alpha\alpha'} \partial_x^2\right) S_{\alpha'\beta}(x,t) + \int_0^t ds \int dy\, \partial_y^2 \underbrace{M_{\alpha\alpha'}(y,s)}_{\text{memory term}} S_{\alpha'\beta}(x-y,t-s) \Big\}$$

$$M_{\alpha\alpha'}(x,t) = 2 \sum_{\beta',\beta'',\gamma',\gamma''=1}^{n} G^{\alpha}_{\beta'\gamma'} G^{\alpha'}_{\beta''\gamma''} S_{\beta'\beta''}(x,t)\, S_{\gamma'\gamma''}(x,t)$$

cubic

- asymptotics
- numerical solutions

$\Rightarrow$ decoupling and exponents, scaling functions, phase diagram

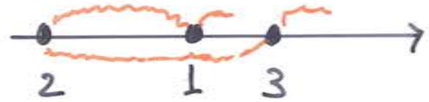
ONLY for covariance

2. anharmonic chains

1D, positions q_j, momenta p_j

$$H = \sum_j \left\{ \tfrac{1}{2} p_j^2 + V(q_{j+1} - q_j) \right\}$$

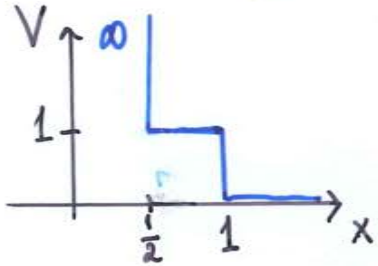
in general, no ordering



examples:

FPU chain: $V(x) = \frac{1}{2} x^2 + \frac{1}{3} a x^3 + \frac{1}{4} b x^4$ "solid"

shoulder:



$q_j \leq q_{j+1}$ "fluid"

Toda: $V(x) = e^{-x}$ integrable

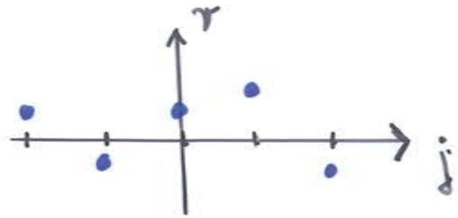
HERE: non-integrable chains

→ stretch

$$r_j = q_{j+1} - q_j \quad \Rightarrow \quad \left\| \begin{aligned} \frac{d}{dt} r_j &= p_{j+1} - p_j \\ \frac{d}{dt} p_j &= V'(r_j) - V'(r_{j-1}) \end{aligned} \right|$$

locally conserved

hamiltonian lattice field theory $\{r_j, p_j\}_{j\in\mathbb{Z}}$



local energy $\quad e_j = \frac{1}{2} p_j^2 + V(r_j)$

$$\frac{d}{dt} e_j = p_{j+1} V'(r_j) - p_j V'(r_{j-1})$$

locally conserved

conserved fields $\quad (r_j, p_j, e_j) = \vec{q}_j$

currents $\quad (-p_j, -V'(r_{j-1}), -p_j V'(r_{j-1})) = \vec{J}(j)$

NO MORE

rules out Toda

equilibrium time correlations

conserved fields $\vec{g}_j = (r_j, p_j, e_j)$

microcanonical $\rightsquigarrow$ canonical

Lagrange P, u, β

pressure, mean velocity, inverse temperature

$$\frac{1}{Z} \prod_j e^{-\beta\left(\frac{1}{2}(p_j - u)^2 + V(r_j) + P r_j\right)}$$

$$-\langle V'(r_j) \rangle_{P,u,\beta} = P$$

---

correlations 3×3 matrix

$$S_{\alpha\beta}(j,t) = \langle g_{j\alpha}(t)\, g_{0\beta}(0) \rangle_{P,u,\beta} - \langle g_{0\alpha} \rangle \langle g_{0\beta} \rangle$$

solution of Newton's equation of motion

$u = 0$

hydronamic approximation slow variation of $\vec{q}_j(t)$

lattice j $\rightsquigarrow$ continuum x

$$(r_j(t),\, p_j(t),\, e_j(t)) \rightsquigarrow (\ell(x,t),\, u(x,t),\, e(x,t))$$

$$\partial_t \ell + \partial_x j_\ell = 0\,, \quad \partial_t u + \partial_x j_u = 0\,, \quad \partial_t e + \partial_x j_e = 0$$

currents by average in local equilibrium

$$(j_\ell, j_u, j_e) = \langle \vec{J}(j) \rangle_{\ell,u,e} = \Big(-u,\ P(\ell, \underbrace{e - \tfrac{1}{2}u^2}_{e_{int}}),\ u P(\ell, \underbrace{e - \tfrac{1}{2}u^2}_{e_{int}})\Big)$$

$u = 0\,, \quad e_{int} = e$

REQUIRES $(P, \beta) \Leftrightarrow (\ell, e_{int})$

expansion at equilibrium

$$(\ell_0 + u_1,\ 0 + u_2,\ e_0 + u_3)$$

uniform background

- linear order

$$\partial_t \vec{u} + \partial_x A \vec{u} = 0$$

3×3 matrix A

equilibrium susceptibility C

depends on ℓ_0, e_0

$$C_{\alpha\beta} = \langle g_{0\alpha}\, g_{0\beta} \rangle_{P,0,\beta} - \langle g_{0\alpha} \rangle \langle g_{0\beta} \rangle$$

$$C > 0$$

$$AC = CA^T$$

transformation R: $R A R^{-1} = \begin{pmatrix} -c & & 0 \\ & 0 & \\ 0 & & c \end{pmatrix}$ $\quad R C R^T = \mathbb{1}$ normalization

c sound speed

normal modes

$$R \vec{u} = \vec{\phi}$$

- add dissipation + noise $\partial_t \vec{u} + \partial_x (A\vec{u} - \partial_x D\vec{u} - B\vec{\xi}) = 0$

linear theory

- include quadratic Euler currents $\frac{1}{2}\sum_{\alpha,\beta=1}^{3} \vec{H}_{\alpha\beta}\, u_\alpha u_\beta$ depends on ℓ_0, e_0

Hessians $H^\gamma_{\alpha\beta} = \partial_{u_\alpha}\partial_{u_\beta} j_\gamma$

- transform to normal modes $\vec{\phi} = R\vec{u}$

⇝ 3-component KPZ

index 0 , $c_0 = 0$ heat mode

index ±1 , $c_\sigma = \sigma c$ sound modes (left + right movers)

special feature $\| \; G^0_{00} = 0 \; \|$ $\|$ non-KPZ

always

predictions

$$\underbrace{R}_{\text{normal mode}}\ \underbrace{S(j,t)}_{\text{anharmonic chain}}\ R^T)_{\alpha\beta} \overset{\text{large } j,t}{\cong} \delta_{\alpha\beta}\, f_\alpha(j,t) \qquad \alpha,\beta = 0, \pm 1$$

- sound ± 1 $\qquad f_\sigma(x,t) = (\lambda_s t)^{-2/3} f_{KPZ}\left((\lambda_s t)^{-2/3}(x - \sigma c t)\right)$

$$\lambda_s = 2\sqrt{2}\, |G^1_{11}|$$

- heat $\quad 0$ $\qquad \hat{f}_0(k,t) = e^{-|k|^{5/3} \lambda_h t}$ $\qquad$ Levy 5/3

λ_h ? $\qquad$ exact solution missing

$\hat{f}_0$?

|| λ_s, λ_h are non-universal coefficients ||

3. MD simulations

- Fermi-Pasta-Ulam $\quad V(r) = \frac{1}{2} r^2 + \frac{1}{3} a r^3 + \frac{1}{4} b r^4$

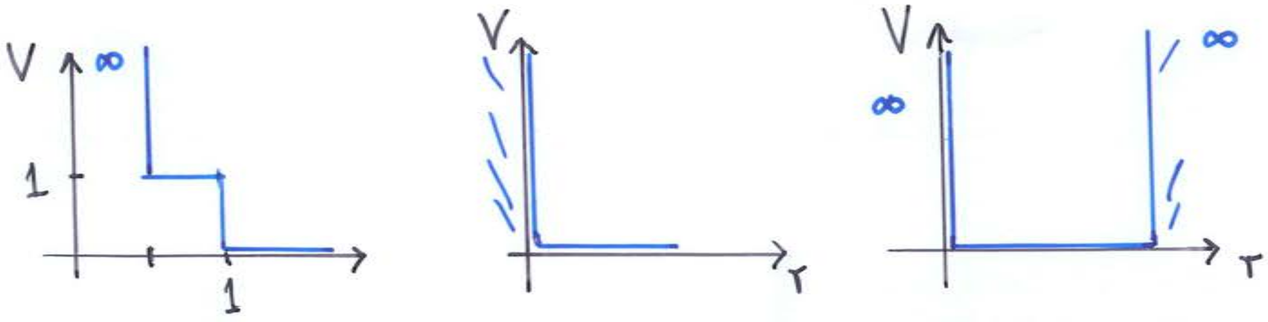
Lepri, Livi, Straka 2014

large β, small a

Dhar et al. 2014

$\beta = 1, \quad a = 2, \quad P = 1$

- hard collisions



shoulder $\qquad$ hard point gas $\qquad$ square well

Mendl, H.S. 2014

$\beta = 1, \; P = 1$

alternating masses $\frac{m_1}{m_0} = 3$ $\qquad$ [$\frac{m_0}{m_1} = 1$ is integrable

- fix V, P, β $\rightsquigarrow$ c, A, C, G, R are computable

symmetry $\quad$ square well $P = 0$

$\rightsquigarrow \quad G^{\alpha}_{\alpha\alpha} = 0, \quad \alpha = 0, \pm 1$

± 1: diffusive, $\quad 0$: Levy $\frac{3}{2}$

- size $N = 10^3 .. 10^4$
- time $t < N/2c \cong 10^3 - 10^4$ up to first collision of sound peaks
- method

random initial configuration, canonical equilibrium, i.i.d.,

evolve by Newton | solve differential eqs.
or collision to collision

conserved fields $g_{i+j\,\alpha}(t)\, g_{i\,\beta}(0)$

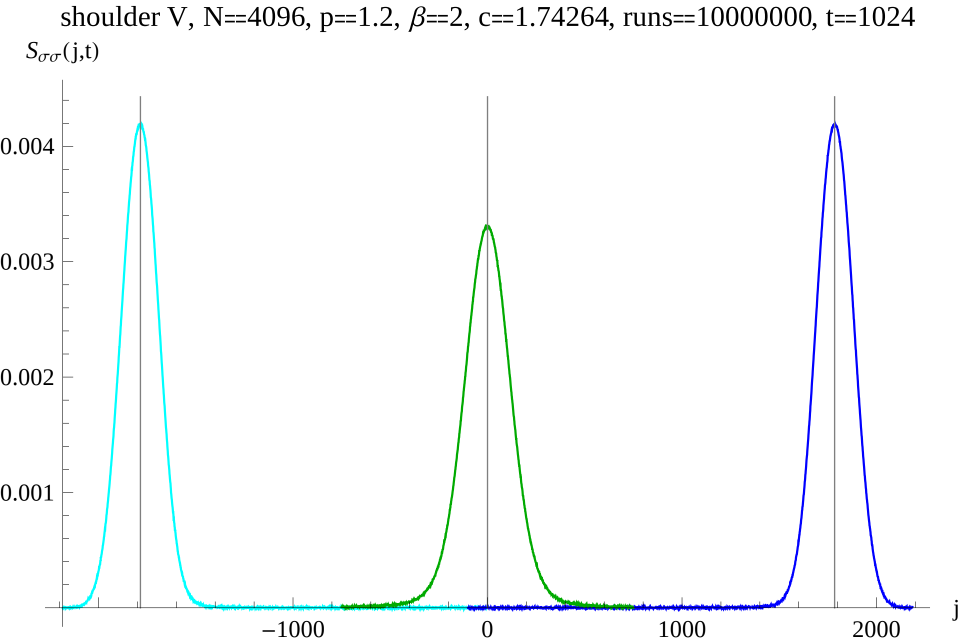
average over $i = 1, .., N$, 10^7 realizations

full 3×3 matrix (maximal resolution in j, minimal in t)

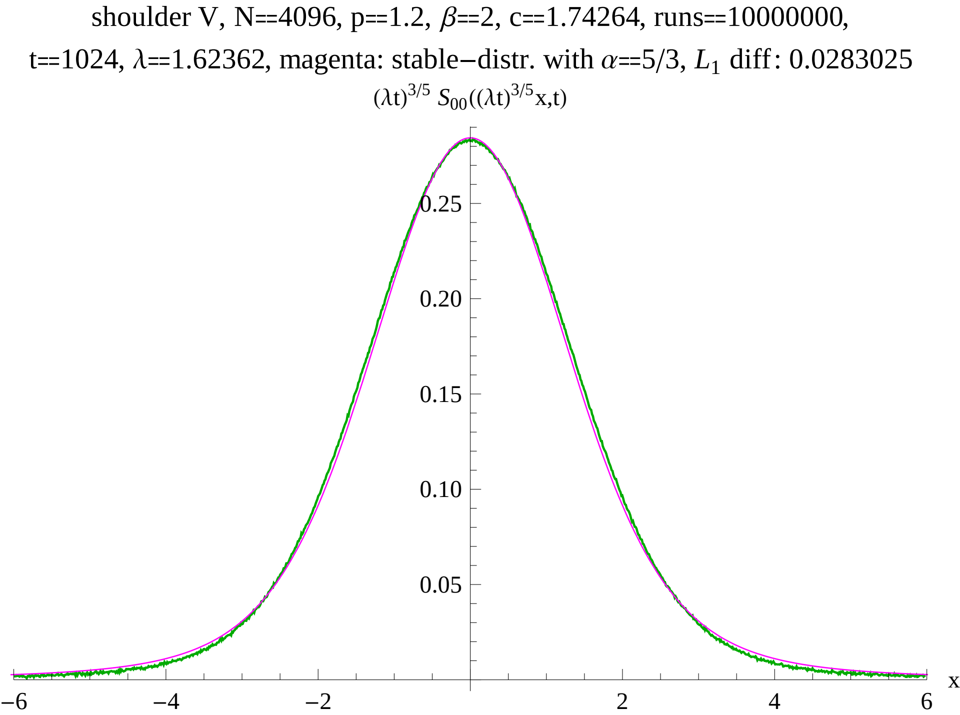
$R\,S(j,t)\,R^T \cong$ diagonal

PLOT $(RSR^{-1})_{00}$ heat

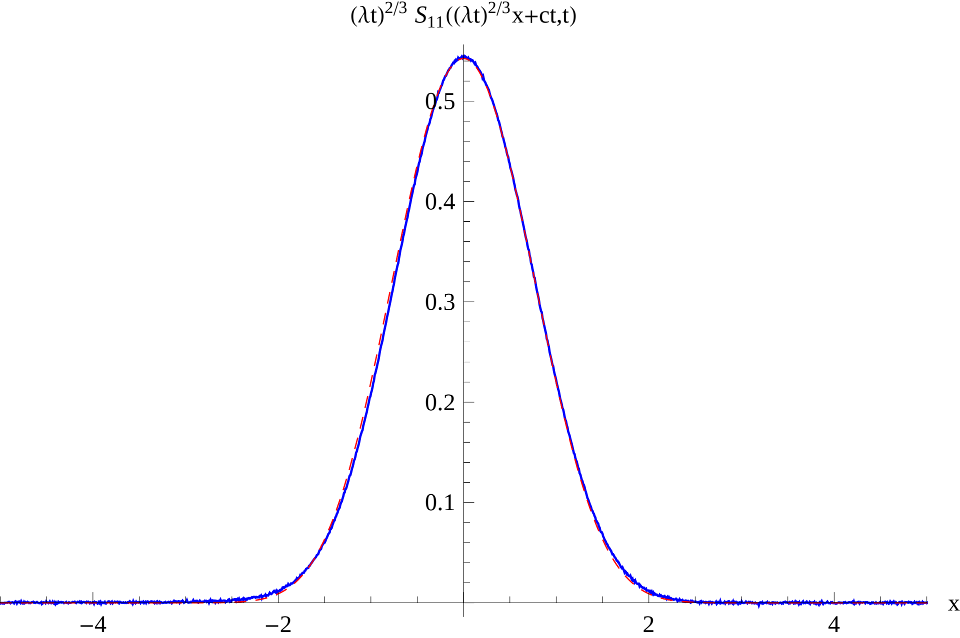
$(RSR^{-1})_{11}$ sound

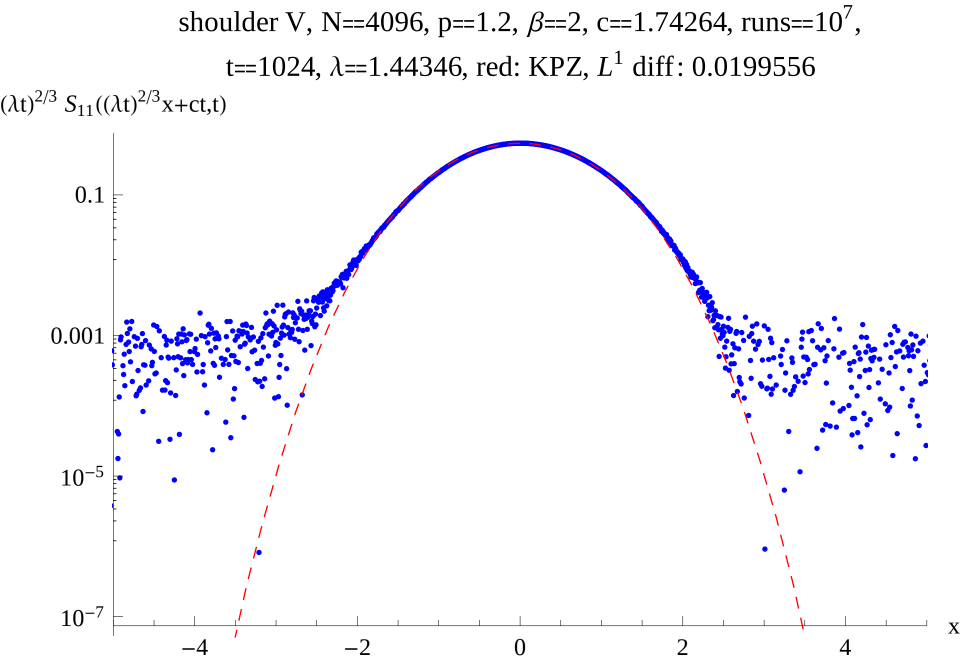


shoulder V, N==4096, p==1.2, β==2, c==1.74264, runs==10000000, t==1024
$S_{\sigma\sigma}$(j,t)
0.004
0.003
0.002
0.001
−1000
0
1000
2000
j

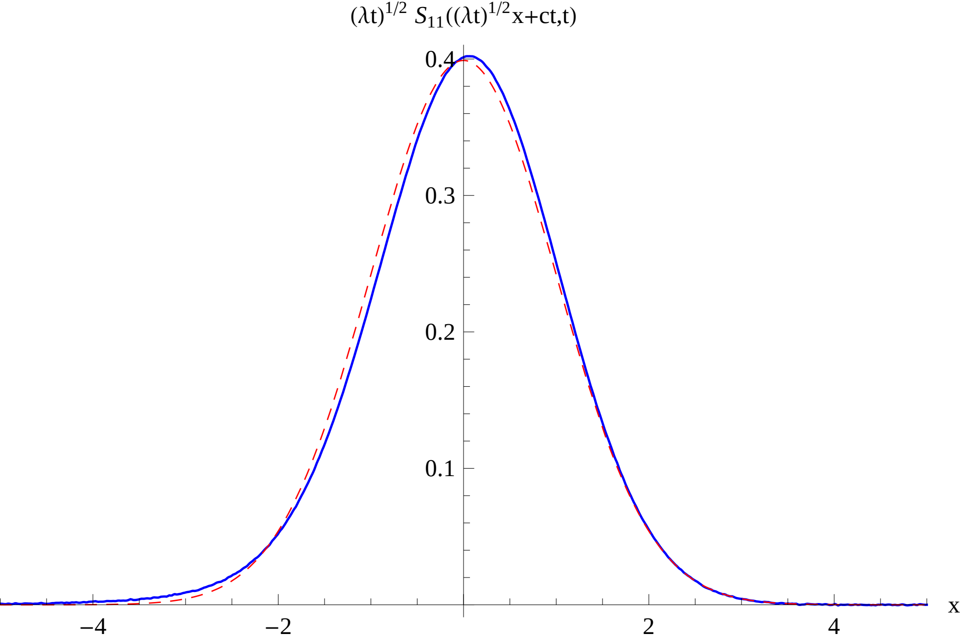

shoulder V, N==4096, p==1.2, β==2, c==1.74264, runs==10000000,
t==1024, λ==1.62362, magenta: stable−distr. with α==5/3, L1 diff: 0.0283025
(λt)^3/5 S00((λt)^3/5x,t)
0.25
0.20
0.15
0.10
0.05
x
−6
−4
−2
2
4
6

shoulder V, N==4096, p==1.2, β==2, c==1.74264, runs==10000000,
t==1024, λ==1.44346, red: KPZ, L_1 diff: 0.0199556

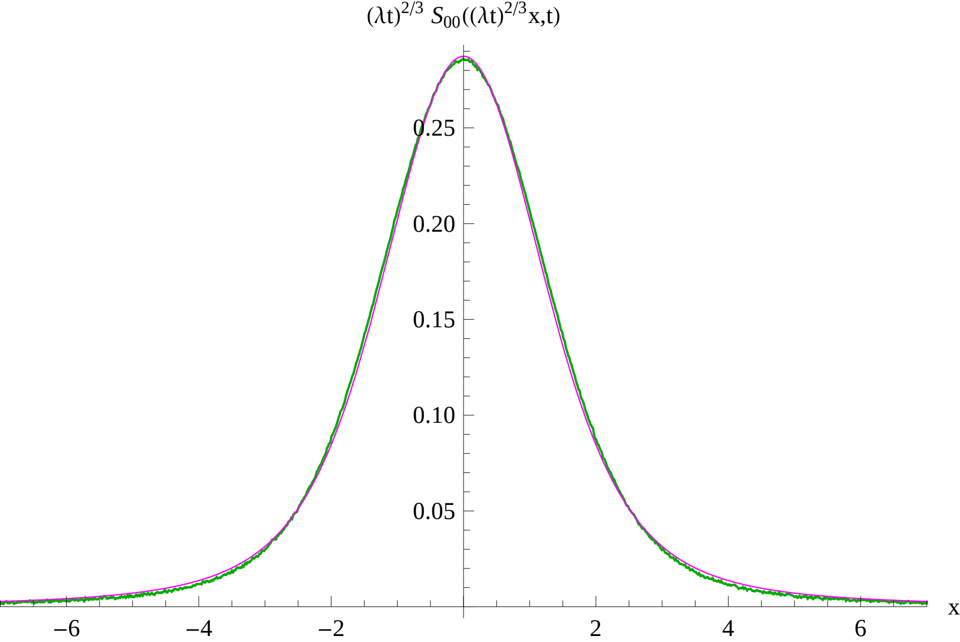


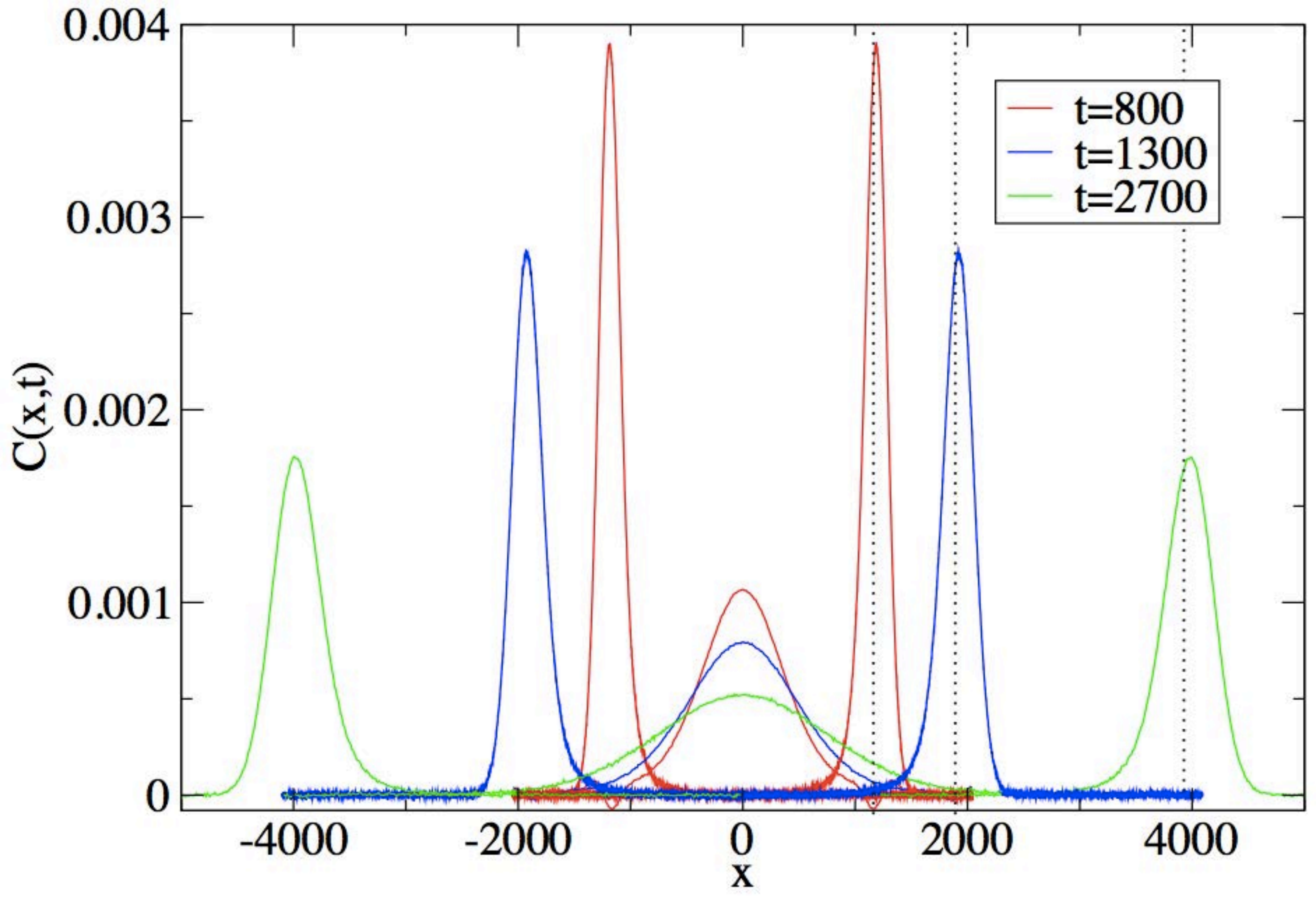

shoulder V, N==4096, p==1.2, β==2, c==1.74264, runs==10^7,
t==1024, λ==1.44346, red: KPZ, L^1 diff: 0.0199556
(λt)^2/3 S_11((λt)^2/3 x+ct,t)
0.1
0.001
10^−5
10^−7
−4
−2
0
2
4
x

square well with a==1, masses m_0==1, m_1==3, N==4096,
p==0, β==2, c==Sqrt[3], runs==10^7, t==1024, λ==4.337,
red: $(2\pi)^{-1/2}$Exp[$-x^2/2$], L^1 diff: 0.0415143

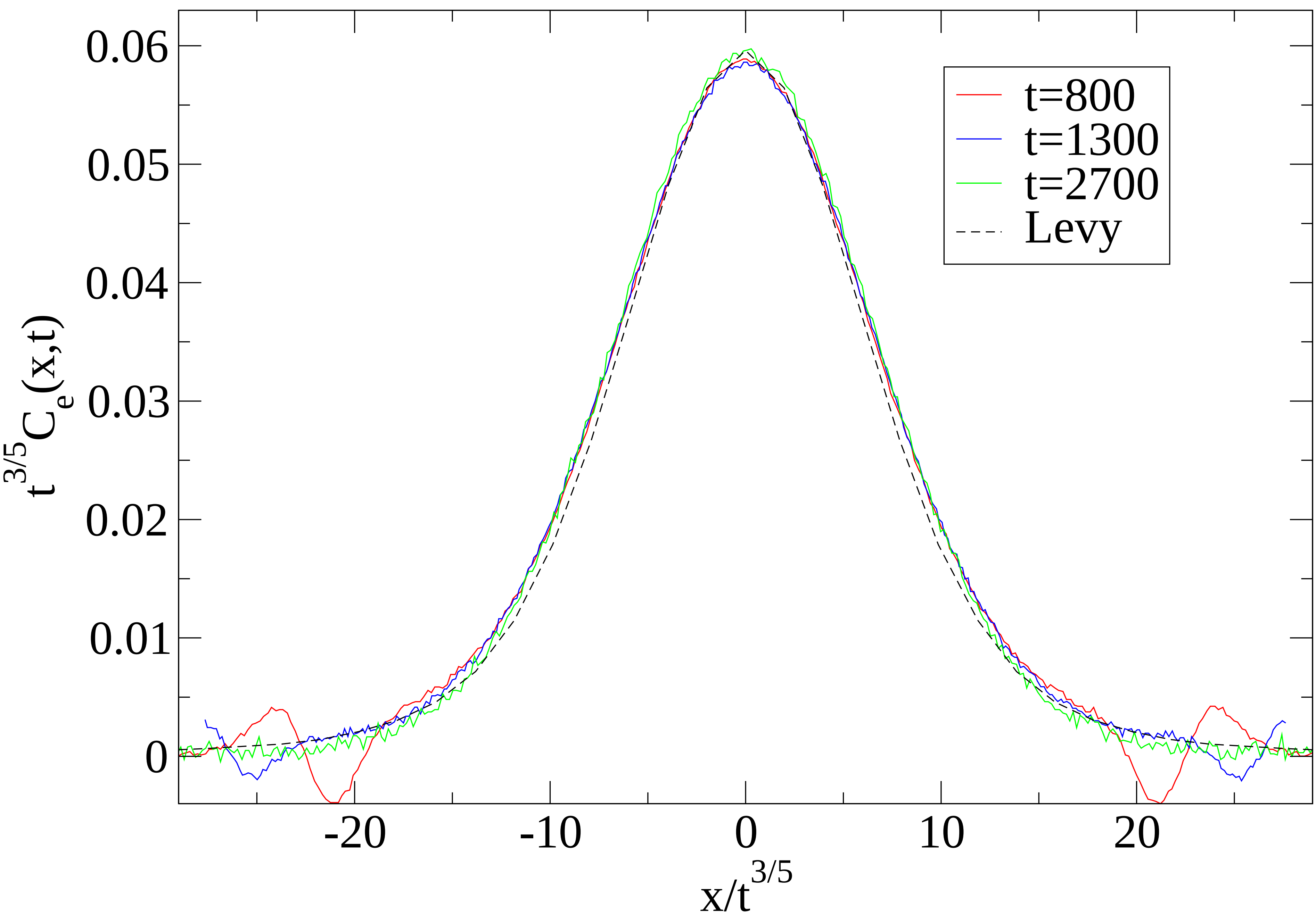


square well with a==1, masses m_0==1, m_1==3, N==4096,
p==0, β==2, c==Sqrt[3], runs==10^7, t==1024, λ==1.32418,
magenta: α−stable−distr. with α==3/2, L^1 diff: 0.025795

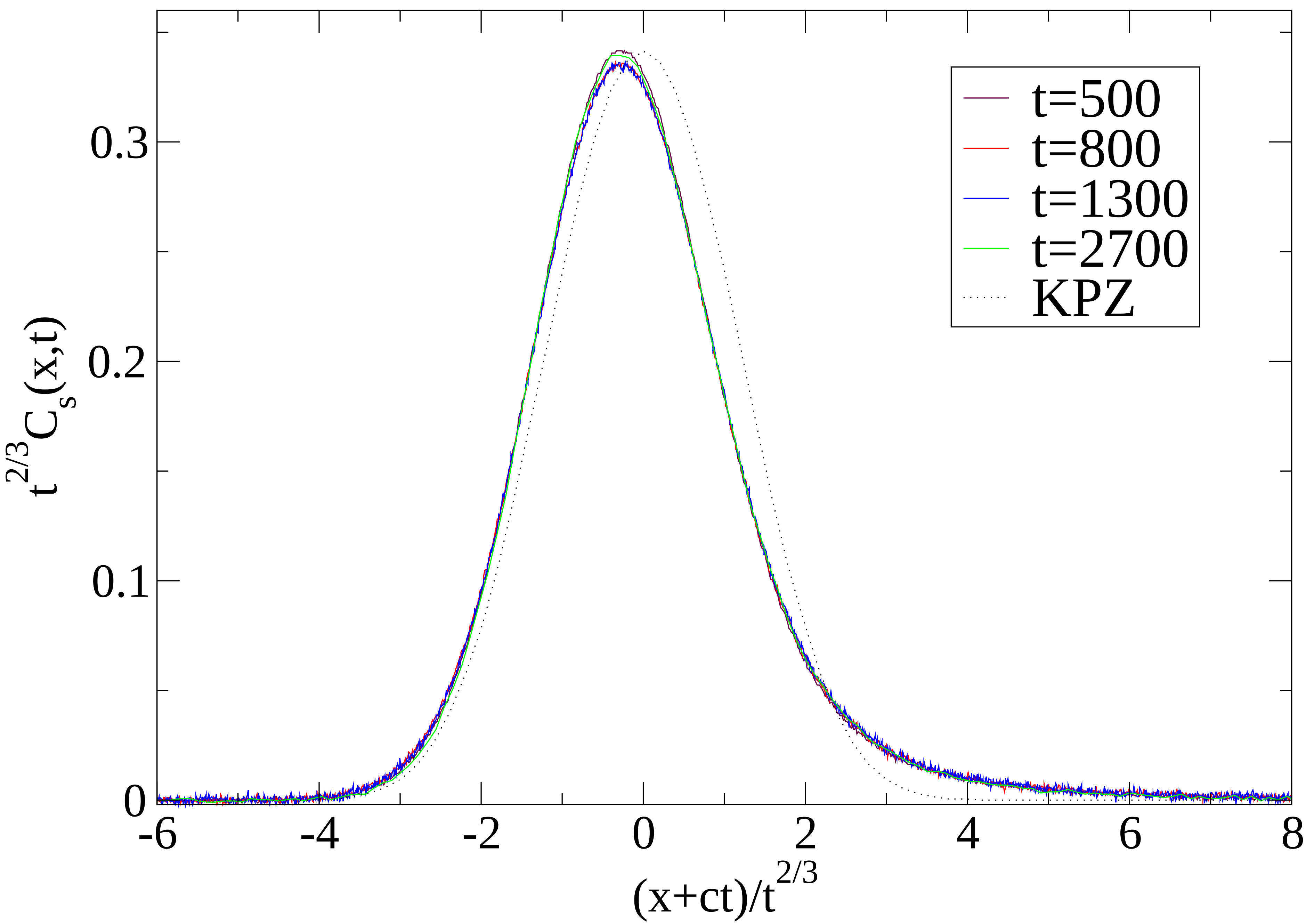




0.004
0.003
0.002
0.001
0
C(x,t)
-4000
-2000
0
2000
4000
x
t=800
t=1300
t=2700



0.06
0.05
0.04
0.03
0.02
0.01
0
-20
-10
0
10
20
$t^{3/5}C_e(x,t)$
$x/t^{3/5}$
t=800
t=1300
t=2700
Levy


t=500
t=800
t=1300
t=2700
KPZ
0.3
0.2
0.1
0
-6
-4
-2
0
2
4
6
8
$t^{2/3}C_s(x,t)$
$(x+ct)/t^{2/3}$

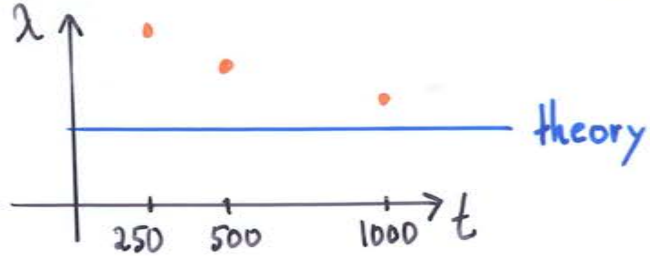
4. Conclusions / outlook

- 1D systems with several conservation laws

  most recent member of the KPZ universality class

- asymptotia has NOT been reached (exceptions)

  non-universal λ is drifting



- better understanding of stochastic PDE

  exact solutions most welcome