Anharmonic Chains

and Nonlinear Fluctuating Hydrodynamics

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joint work with

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setting the stage: equilibrium time correlations of classical fluids

$$H = \sum_j \tfrac{1}{2} p_j^2 + \tfrac{1}{2} \sum_{i \neq j} V(q_i - q_j)$$ short range, stable V

- equilibrium $\langle p_j \rangle = 0$, β, μ
- $t=0$, small perturbations at 0

$$\Longleftrightarrow \quad \langle A(t)\, B(0) \rangle_{\beta,\mu} - \langle A \rangle_{\beta,\mu} \langle B \rangle_{\beta,\mu}$$

response perturbation

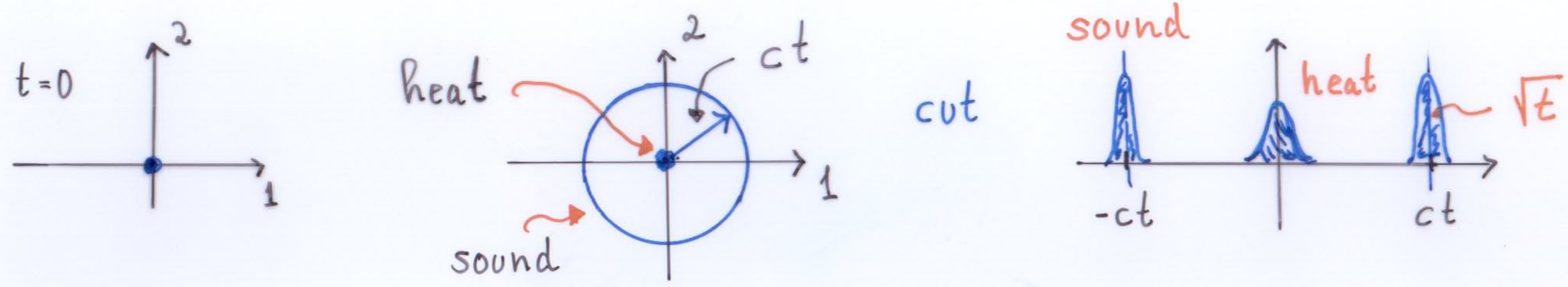
dealt with by

- linear fluctuating hydrodynamics — Landau, Lifshitz 1959

|| Gaussian fluctuation theory ||

earlier work

Einstein 1910, Onsager, ...



thermodynamics: speed of sound c, Landau Placzek ratios

- diffusive $\sqrt{t}$ spreading: transport coefficients

  long time tails in Green-Kubo $t^{-d/2}$ ⇝ dimension $d \geq 3$

  $d = 2 \quad (t \log t)^{1/2}$ Resibois, de Leener 1977

// What about $d = 1$? //

- super diffusive
- non linear Euler currents
- non integrable system

outline

1. anharmonic chains, lattice field theory

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

2. nonlinear fluctuating hydrodynamics PART I

3. MD simulations

4. PART II

5. conclusions

1. anharmonic chain

stretch $r_j = q_{j+1} - q_j$

$$\frac{d}{dt} r_j = p_{j+1} - p_j$$

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

conserved fields

periodic b.c.

pressure

equilibrium $\{r_j, p_j\}$ i.i.d. $\quad \frac{1}{Z} e^{-\beta(p_j - u)^2/2} \times \frac{1}{Z} e^{-\beta(V(r_j) + P r_j)}$

3 conserved fields $r_j,\ p_j,\ e_j = \frac{1}{2} p_j^2 + V(r_j) = \vec{g}_j$ NO MORE

equilibrium time correlations

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

mean velocity $= 0$

claim $\quad 3 \times 3$ transformation matrix R (acting on components)

thermodynamics

$$R S(j,t) R^{-1} \cong \text{diagonal}$$

heat $\quad (R S(j,t) R^{-1})_{00}$ mean 0, width $t^{3/5}$

sound $\quad (R S(j,t) R^{-1})_{\sigma\sigma}$ mean $\sigma c t$, width $t^{2/3}$ $\quad \sigma = \pm 1$

generic case

phase diagram

2. nonlinear fluctuating hydrodynamics PART I

Euler scale, local equilibrium

fields $u_\alpha(x,t)$, $\alpha = 1,2,3$

particle label j

$$\partial_t u_\alpha + \partial_x j_\alpha(\vec{u}) = 0$$

$j_1 = -\langle p_0 \rangle$, $j_2 = -\langle V'(r_0) \rangle$, $j_3 = -\langle p_0 V'(r_{-1}) \rangle$

BASIC assumptions:

- expand currents up to second order
- add dissipation + noise

$$\rightsquigarrow \quad j_\alpha(\vec{u}) = (A\vec{u})_\alpha + \langle \vec{u}, H^\alpha \vec{u} \rangle - \partial_x (D\vec{u})_\alpha + (B\xi)_\alpha$$

diffusion

white noise in x,t

fluctuation-dissipation

- equilibrium susceptility C

$$AC = CA^T$$

$$DC + CD = BB^T$$

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

$R A R^{-1} = \mathrm{diag}(-c, 0, c)$ and $R C R^{T} = 1$ determines R

$2D = BB^{T}$

$\Rightarrow$ $\partial_t \phi_\alpha + \partial_x \left(c_\alpha \phi_\alpha + \langle \vec{\phi}, G^\alpha \vec{\phi} \rangle - \partial_x (D\phi)_\alpha + (B\xi)_\alpha \right) = 0$, $\alpha = \pm 1, 0$

- D, B fix the measure, large scale does not depend on this choice
- broadening of the peaks depends on G^α
- relevant couplings $G^\alpha_{\beta\beta}$
- $G^0_{00} = 0$ always special

$\Rightarrow$ add boundary conditions (in principle)

- decoupling argument for $\alpha \neq \beta$ $\quad \phi_\alpha(x,t)\,\phi_\beta(x,t) \simeq 0$

$$\rightsquigarrow \quad \partial_t \phi_1 + \partial_x \left(c\,\phi_1 + G^1_{11}\,\phi_1^2 - \tfrac{1}{2} D_{11}\,\phi_1 + B_{11}\,\xi_1 \right) = 0$$

$\Rightarrow$ IF $G^1_{11} \neq 0$, stochastic Burgers alias 1D KPZ equation

stationary!

$$\langle \phi_1(x,t)\,\phi_1(0,0) \rangle = (\lambda_1 t)^{-2/3} f_{\mathrm{KPZ}}\left((x - ct)(\lambda_1 t)^{-2/3} \right)$$

$f_{\mathrm{KPZ}} \geqslant 0$, $f_{\mathrm{KPZ}}(x) = f_{\mathrm{KPZ}}(-x)$, $\int dx\, f_{\mathrm{KPZ}}(x) = 1$

$\lambda_1 = 2\sqrt{2}\,|G^1_{11}|$

BUT $G^0_{00} = 0$ always

} nonuniversal

$$\langle \phi_0(x,t)\,\phi_0(0,0) \rangle = (\lambda_0 t)^{-3/5} f_{\mathrm{Levy}\,\frac{5}{3}}\left(x\,(\lambda_0 t)^{-3/5} \right)$$

symmetric $\frac{5}{3}$ stable distribution

3. MD simulations

Lepri, Livi, Straka 2014

Dhar et al. 2014

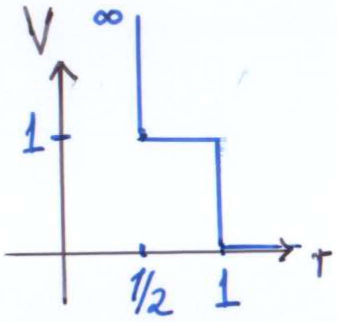
- Fermi-Pasta-Ulam FPU $V(r) = \frac{1}{2} r^2 + \frac{1}{3} a r^3 + \frac{1}{4} b r^4$

fixed β, P

- hard collisions

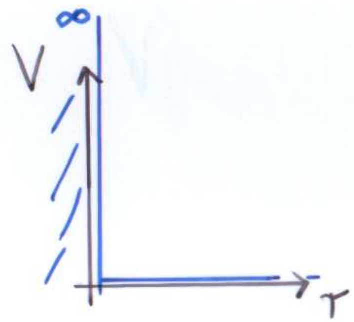
Mendl, HS 2014 ‖ van Beijeren, Posch 2014

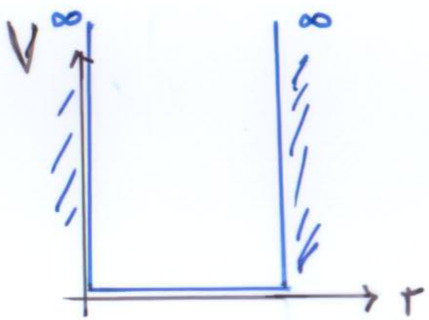
— shoulder potential



also attractive

— hard core





alternating masses

$m_{2j} = m_0, \quad m_{2j+1} = m_1, \quad \frac{m_1}{m_0} = 3$

$\frac{m_1}{m_0} = 1$ integrable

- size: $N = 10^3 \dots 10^4$

$r_1 = r_{N+1}$, $p_1 = p_{N+1}$

- time: $t < N/2c \cong 10^3 \dots 10^4$ first collision

- method: random initial configuration, evolve by Newton

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

  average over i, 10^7 realizations

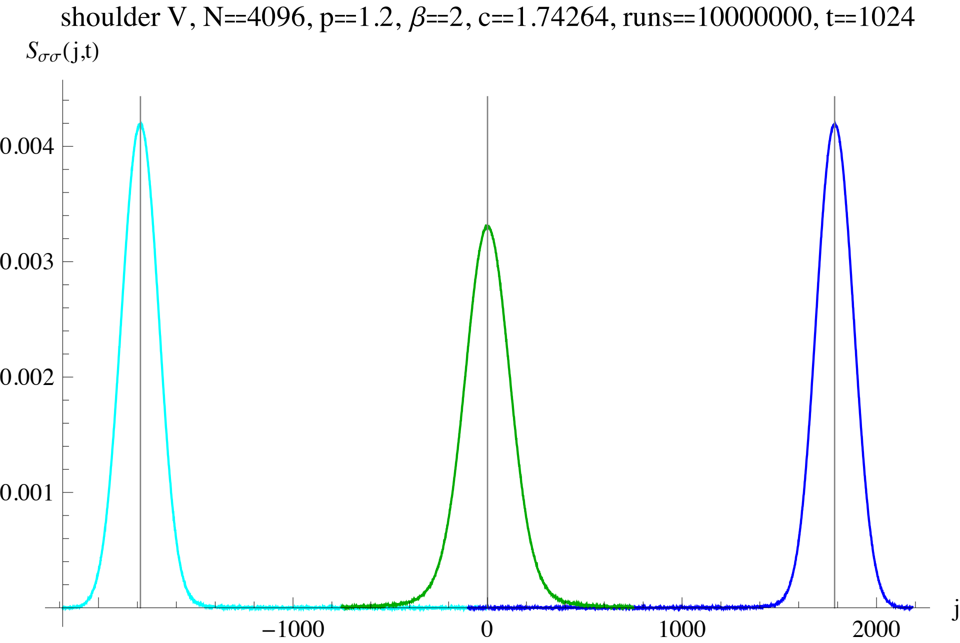
full 3×3 matrix $\Updownarrow$ $\left.\begin{array}{l}\text{maximal resolution in } j \\ \text{low resolution in } t\end{array}\right\}$

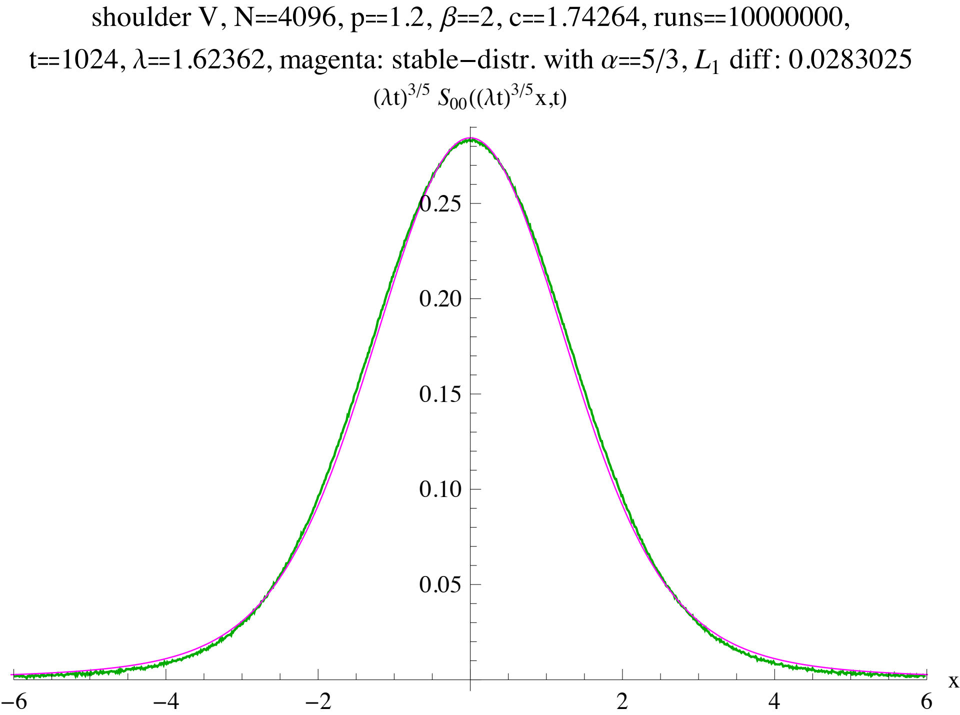
C, R, G sound speed c from theory up to 3^{rd} cumulants in r, $V(r)$

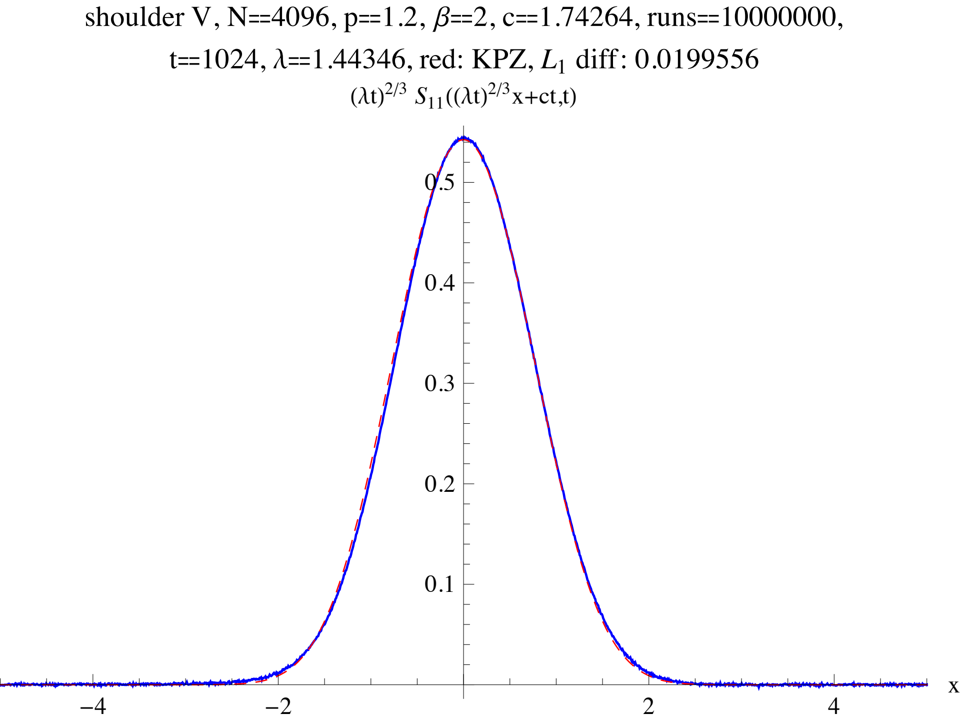
$R\,S(j,t)\,R^{-1} \cong$ diagonal

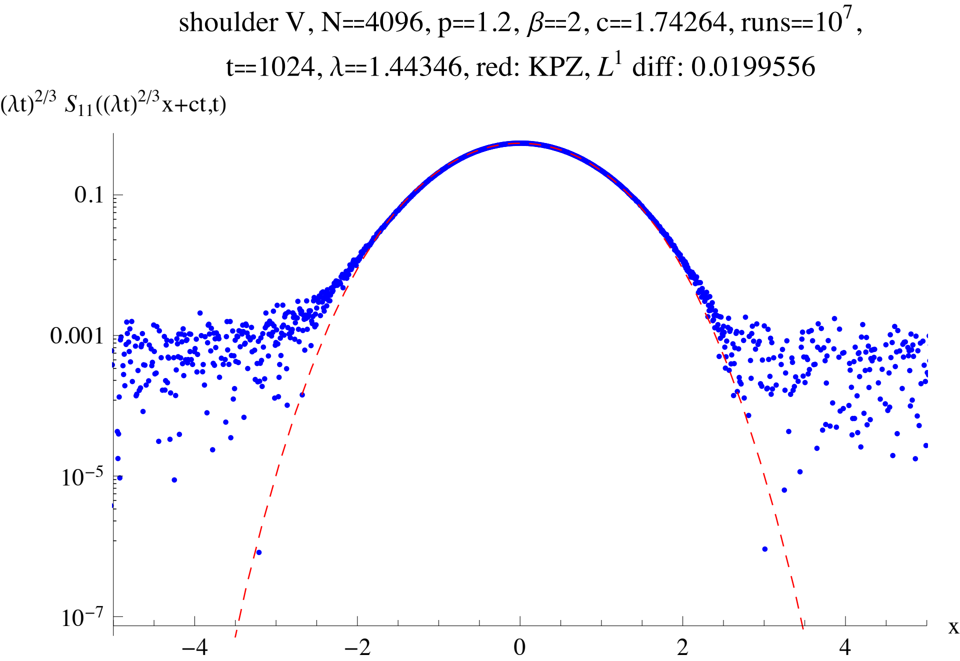
PLOT $(R\,S\,R^{-1})_{00}$ heat

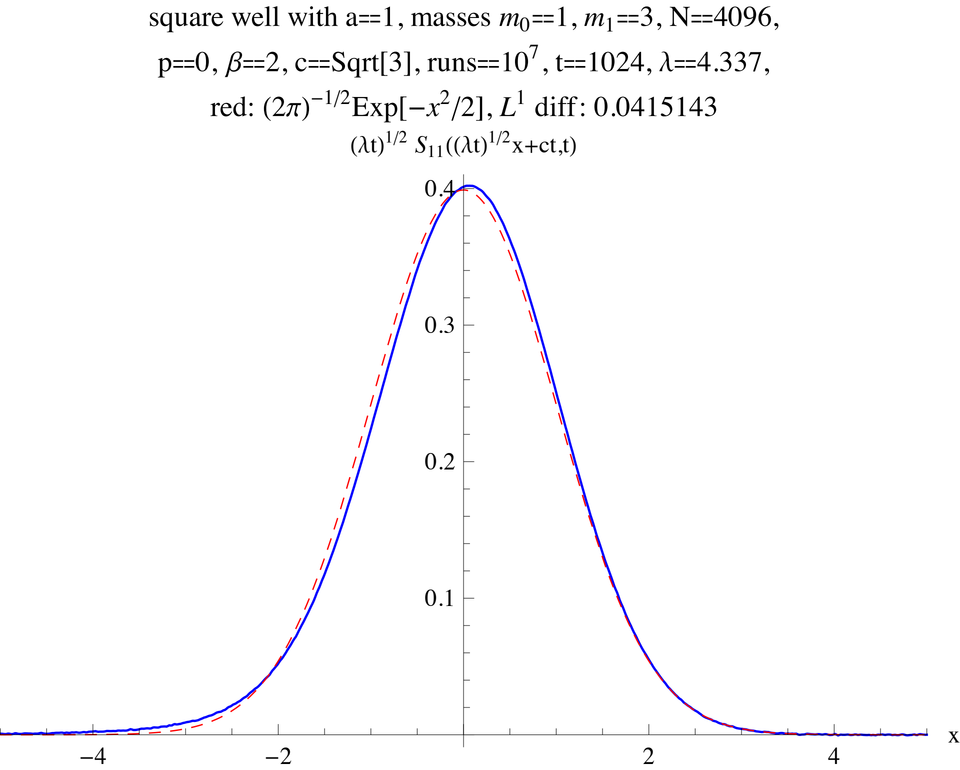
$(R\,S\,R^{-1})_{11}$ sound

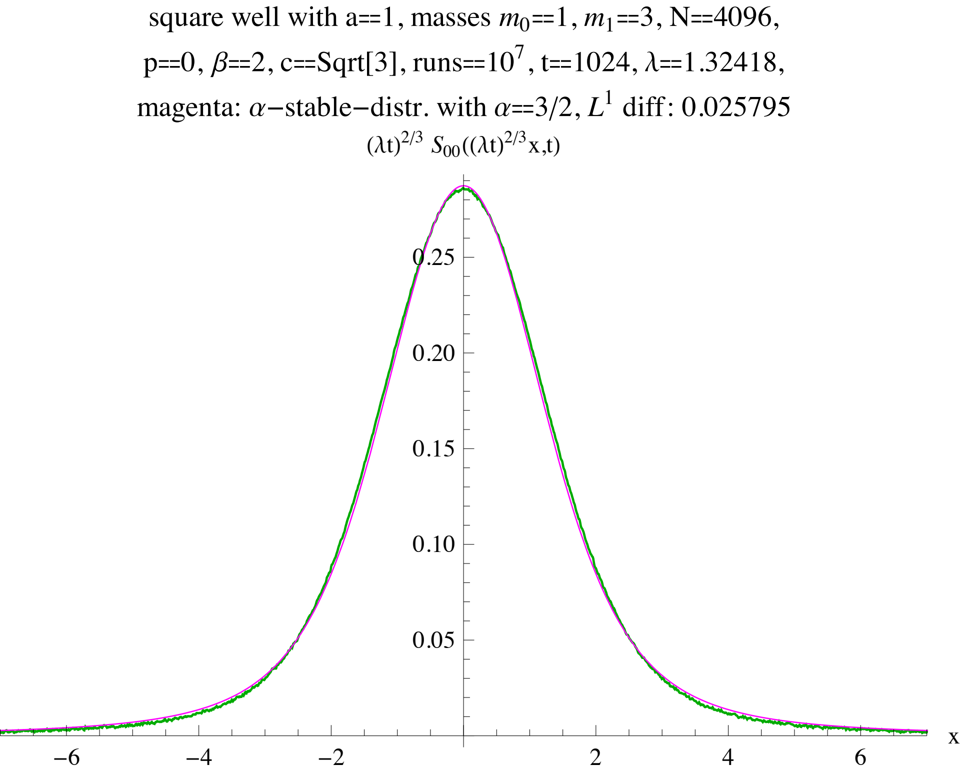

shoulder V, N==4096, p==1.2, β==2, c==1.74264, runs==10000000, t==1024
$S_{\sigma\sigma}(j,t)$
0.004
0.003
0.002
0.001
−1000
0
1000
2000
j

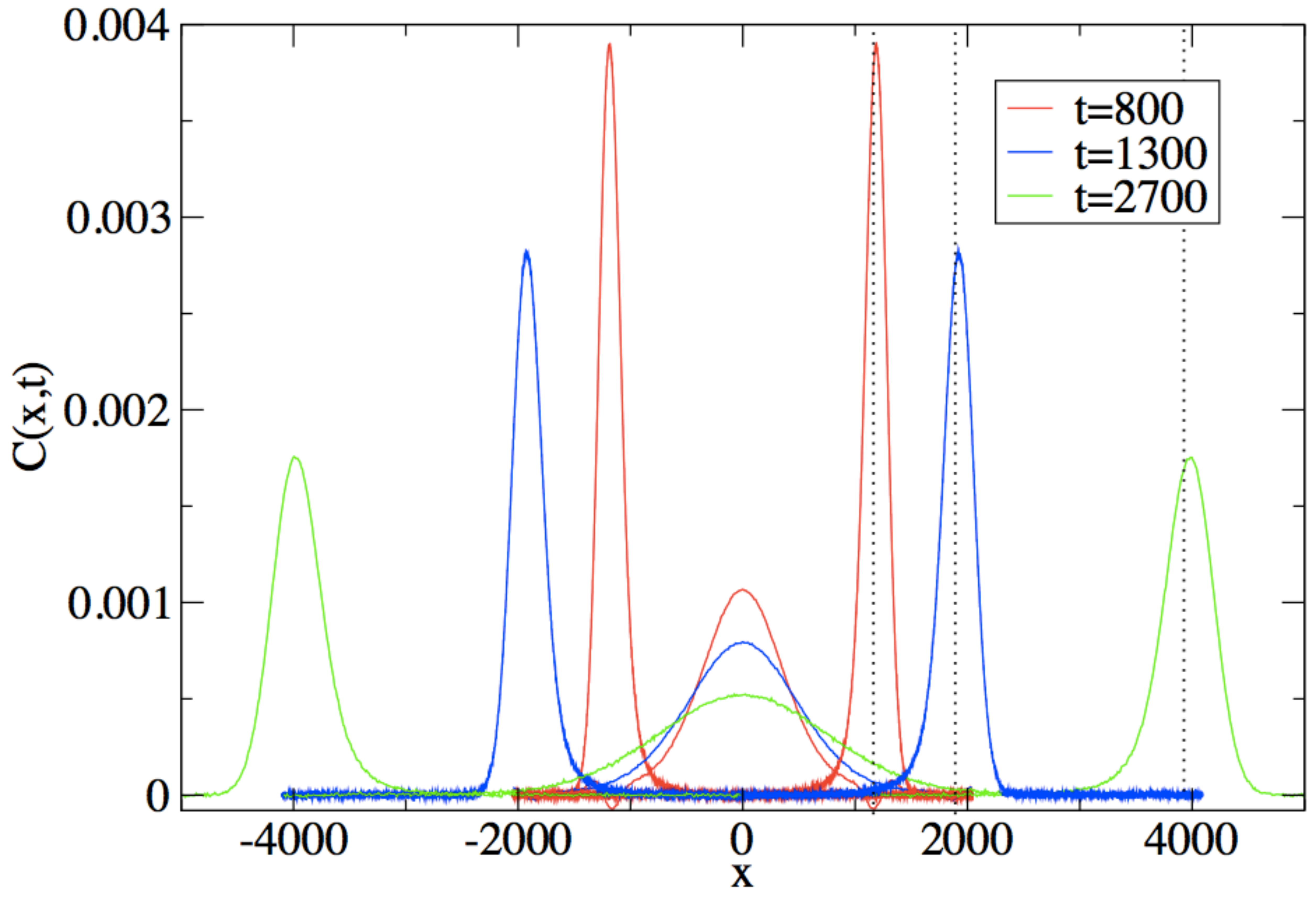

shoulder V, N==4096, p==1.2, β==2, c==1.74264, runs==10000000,
t==1024, λ==1.62362, magenta: stable−distr. with α==5/3, L1 diff: 0.0283025
(λt)^3/5 S00((λt)^3/5 x,t)
0.25
0.20
0.15
0.10
0.05
x
−6
−4
−2
2
4
6

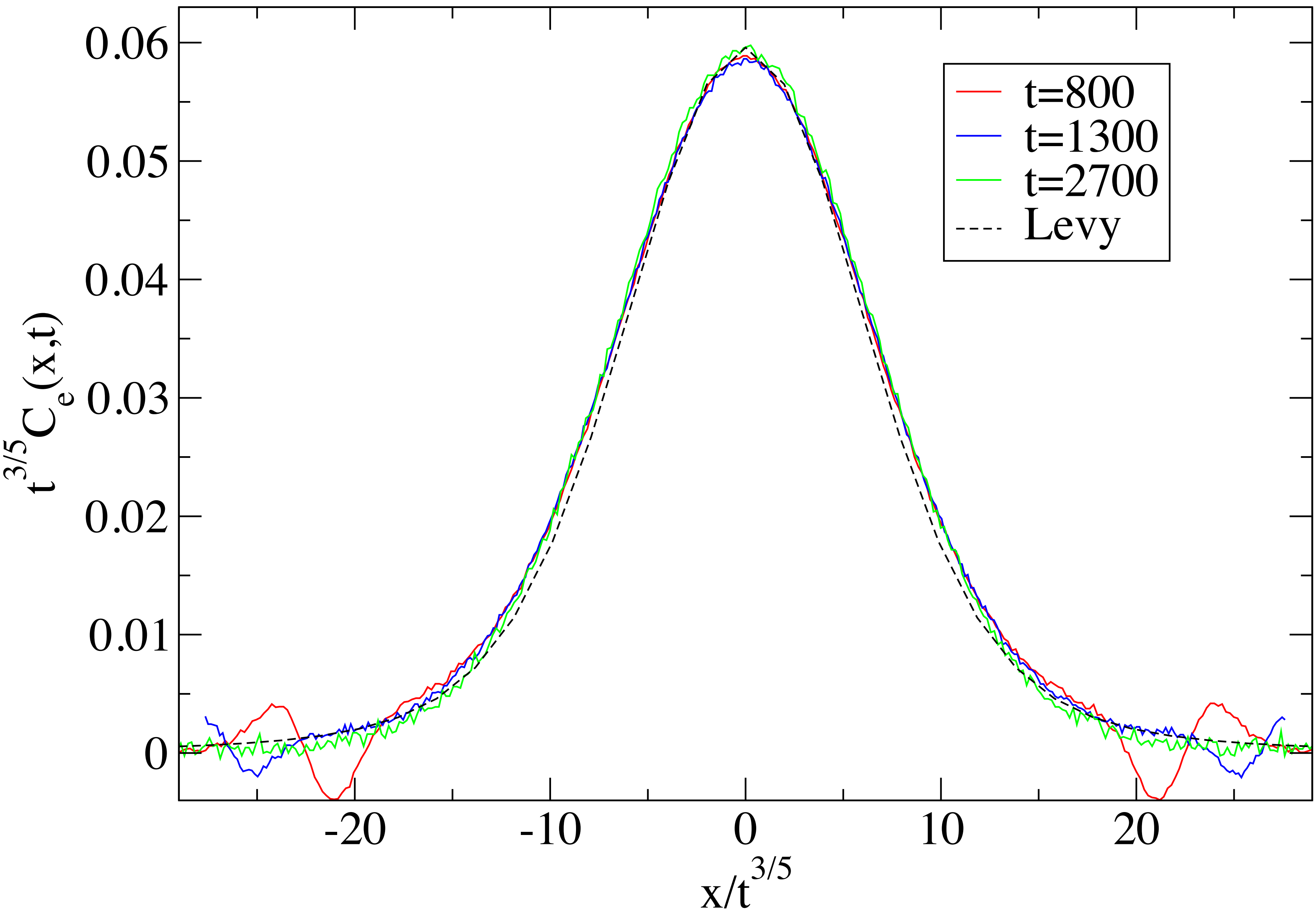

shoulder V, N==4096, p==1.2, β==2, c==1.74264, runs==10000000,
t==1024, λ==1.44346, red: KPZ, L_1 diff: 0.0199556
$(\lambda t)^{2/3}\, S_{11}((\lambda t)^{2/3}x+ct,t)$
0.5
0.4
0.3
0.2
0.1
−4
−2
2
4
x


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

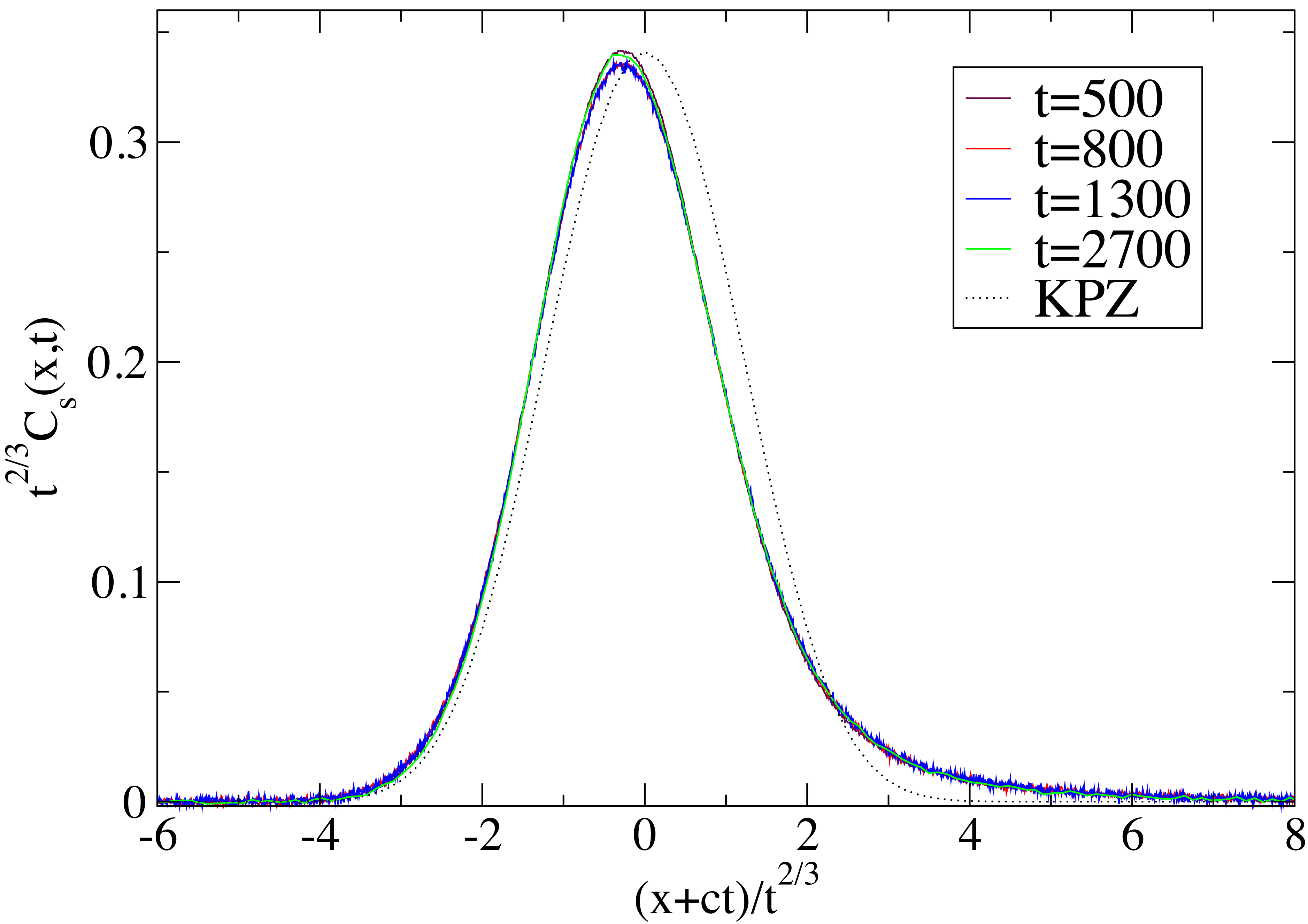

square well with a==1, masses m_0==1, m_1==3, N==4096,
p==0, β==2, c==Sqrt[3], runs==10^7, t==1024, λ==4.337,
red: $(2\pi)^{-1/2}$Exp[$-x^2/2$], L^1 diff: 0.0415143
$(\lambda t)^{1/2}$ $S_{11}((\lambda t)^{1/2}x+ct,t)$
0.4
0.3
0.2
0.1
−4
−2
2
4
x


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==1.32418,
magenta: α−stable−distr. with α==3/2, L^1 diff: 0.025795
$(\lambda t)^{2/3}\ S_{00}((\lambda t)^{2/3}x,t)$
0.25
0.20
0.15
0.10
0.05
−6
−4
−2
2
4
6
x


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



t=800
t=1300
t=2700
Levy
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=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. fluctuating hydrodynamics PART II

ONLY proof : discretized version of

Komorowski, Milton, Olla 2014

3 modes

$$\partial_t \phi_\sigma + \partial_x \left(\sigma c \phi_\alpha - \partial_x \phi_\sigma + \xi_\sigma \right) = 0 \quad , \sigma = \pm 1$$

Bernardin, Goncalves, Milton 2014

$$\partial_t \phi_0 + \partial_x \left(\phi_1^2 - \phi_{-1}^2 - \partial_x \phi_0 + \xi_0 \right) = 0$$

2 modes

⇒ sound: diffusive ; heat: Levy $\frac{3}{2}$

	modes
• symmetric	3
• maximally asymmetric	2

→ a single exact solution fixes non-universal space-time scales ‖

• all other theoretical predictions rely on mode-coupling theory ξ

one - loop approximation

f_{KPZ} is exact ‖ $f_{Levy\,\frac{5}{3}}$ could be exact

- diagonal approximation $\langle \phi_\alpha(x,t)\, \phi_\beta(0,0) \rangle = \delta_{\alpha\beta}\, f_\alpha(x,t)$

  $\alpha, \beta = 0, \pm 1$

- memory equation

$$\partial_t f_\alpha = - c_\alpha \partial_x f_\alpha + D_\alpha \partial_x^2 f_\alpha + \int_0^t ds \int dy\, f_\alpha(x-y, t-s)\, \partial_y^2 M_{\alpha\alpha}(y,s)$$

- memory kernel

$$M_{\alpha\alpha}(x,t) = 2 \sum_{\beta,\gamma = 0,\pm 1} \left| G^\alpha_{\beta,\gamma} \right|^2 f_\beta(x,t)\, f_\gamma(x,t)$$

- initial conditions

$$f_\alpha(x,0) = \delta(x)$$

5. Conclusions / outlook

- nonlinear fluctuating hydrodynamics captures large scale time-correlations
- stochastic models: asymptotia is reached
- mechanical particle systems: asymptotia is not reached
  BUT only for non-universal λ
- applicable to 1D quantum fluids
- a better mathematical understanding of the stochastic PDE
  most welcome