Searching for the Tracy-Widom Distribution in Nonequilibrium Processes

(joint work with Herbert Spohn)

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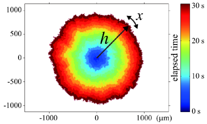
Outline and general concepts

Multiple scales:

- microscopic FPU-type chains (molecular dynamics)
- mesoscopic KPZ partial differential equation
- macroscopic fluid dynamics (hyperbolic conservation laws)

$\rightsquigarrow$ Uncover statistical Tracy-Widom distribution in one-dimensional particle systems



FPU-type anharmonic chains

Particles with positions q_j and momenta p_j
Hamiltonian:

$$H = \sum_j \frac{1}{2m} p_j^2 + V(q_{j+1} - q_j)$$

Interaction potential depends only on difference $q_{j+1} - q_j \rightsquigarrow$ momentum conservation

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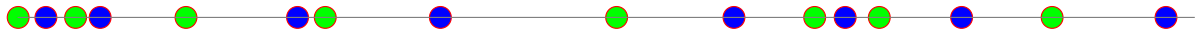
Equations of motion

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} r_j &= \frac{1}{m}(p_{j+1} - p_j) \\ \frac{\mathrm{d}}{\mathrm{d}t} p_j &= V'(r_j) - V'(r_{j-1}) \end{aligned}$$

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



FPU-type anharmonic chains: Conserved fields

Conserved fields:

$$\vec{g}(j) = \begin{pmatrix} r_j \\ p_j \\ e_j \end{pmatrix} \quad \begin{matrix} \text{stretch} \\ \text{momentum} \\ \text{energy} \end{matrix}$$

with stretch $r_j = q_{j+1} - q_j$ and energy $e_j = \frac{1}{2m} p_j^2 + V(r_j)$

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Microscopic currents

$$\vec{\mathcal{J}}(j) = \begin{pmatrix} -\frac{1}{m} p_j \\ -V'(r_{j-1}) \\ -\frac{1}{m} p_j V'(r_{j-1}) \end{pmatrix}$$

$\rightsquigarrow$ microscopic conservation law

$$\frac{\mathrm{d}}{\mathrm{d}t} \vec{g}(j,t) + \vec{\mathcal{J}}(j+1,t) - \vec{\mathcal{J}}(j,t) = 0$$

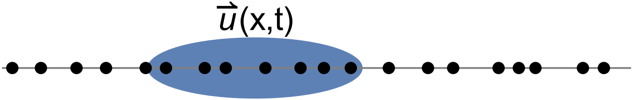
Local thermodynamic equilibrium

Canonical ensemble distribution depending on
inverse temperature β, pressure P and average momentum ν:

$$\frac{1}{Z}\exp\left[-\beta\left(\frac{1}{2m}\left(p_j-\nu\right)^2+V(r_j)+P r_j\right)\right]\mathrm{d}p_j\,\mathrm{d}r_j$$

$\rightsquigarrow$ r_j, p_j are independent (ensemble distribution factorizes)

Using integration by parts: $P = -\langle V'(x)\rangle_{P,\beta}$



$\vec{u} = (r, \nu, \mathfrak{e})$, with total energy $\mathfrak{e} = e + \frac{1}{2}\nu^2$

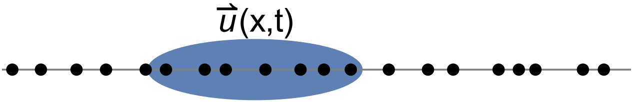
From microscopic to macroscopic conservation laws

microscopic $\frac{\mathrm{d}}{\mathrm{d}t} g_\alpha(j,t) + \mathcal{J}_\alpha(j+1,t) - \mathcal{J}_\alpha(j,t) = 0$

$$\downarrow$$

macroscopic $\partial_t u_\alpha(x,t) + \partial_x \mathrm{j}_\alpha(\vec{u}(x,t)) = 0$

$\vec{u} = (r, \nu, \mathfrak{e})$ and $\alpha = 1, 2, 3$.



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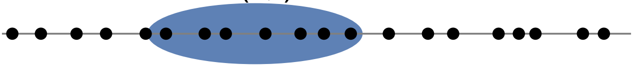

Macroscopic Euler currents: (local) thermal averages of the microscopic currents:

$$\vec{\mathrm{j}}(r, \nu, \mathfrak{e}) = \langle \vec{\mathcal{J}} \rangle_{P,\nu,\beta} = \left(-\nu, P(r, \mathfrak{e} - \tfrac{1}{2}\nu^2), \nu P(r, \mathfrak{e} - \tfrac{1}{2}\nu^2)\right)$$

From hydrodynamics to KPZ

Generic Euler equation (hyperbolic conservation law)

$$\partial_t \tilde{u}(x,t) + \partial_x \mathrm{j}(\tilde{u}(x,t)) = 0$$

Expand current to *second* order in u, add dissipation plus noise $\rightsquigarrow$ Langevin (stochastic Burgers) equation

$$\partial_t u(x,t) + \partial_x \Big(\underbrace{\mathrm{j}'(\bar{u})}_{\text{velocity } c} \; u + \underbrace{\tfrac{1}{2}\mathrm{j}''(\bar{u}) u^2}_{\text{nonlinear current}} - \underbrace{D \partial_x u}_{\text{dissipation}} + \underbrace{\xi}_{\text{noise}} \Big) = 0,$$

where $\xi(x,t)$ is space-time white noise.

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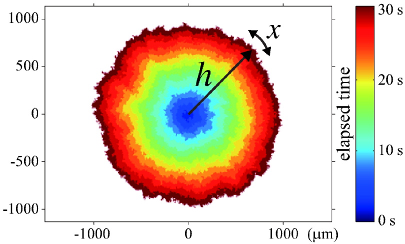
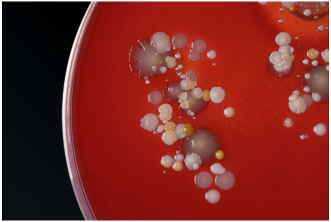
Interpret as derivative of height function: $u(x,t) = \partial_x h(x,t)$
$\rightsquigarrow$ KPZ equation

Kardar-Parisi-Zhang (KPZ) and 1D surface growth

Growing interfaces described by the Kardar-Parisi-Zhang equation



Growing interfaces of liquid-crystal turbulence (Takeuchi and Sano 2010; Takeuchi et al. 2011)

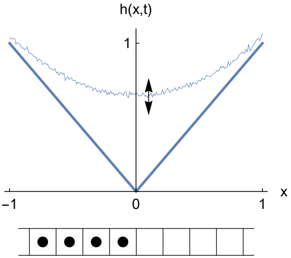


Bacteria growth (APS Physics, Yunker et al. 2013)

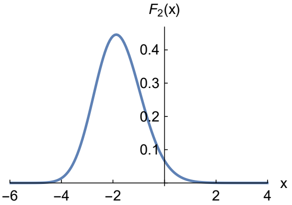
Kardar Parisi Zhang (1986)

$$\partial_t h(x,t) = \underbrace{\tfrac{1}{2}\lambda(\partial_x h)^2}_{\text{tilt-dependent growth}} + \underbrace{D\partial_x^2 h}_{\text{dissipation}} + \underbrace{\xi}_{\text{noise}}$$

Tracy-Widom distribution for wedge initial geometry



$\rightsquigarrow$



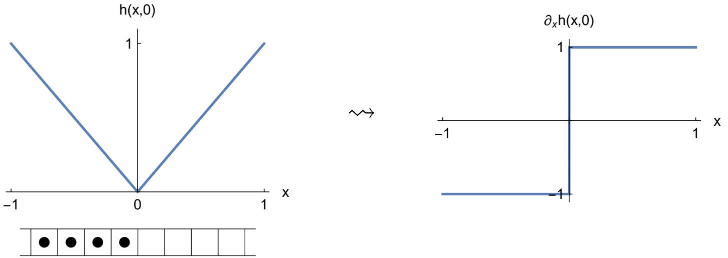
(T)ASEP particle process: integrated current $\Phi(x,t)$ corresponds to height function $h(x,t)$, converges to GUE Tracy-Widom distribution $F_2(x)$:

$$\Phi(0,t) \simeq \frac{1}{4}t - \left(2^{-4}t\right)^{1/3} \xi_{\mathrm{TW}}$$

(Johansson 2000 for TASEP, Tracy and Widom 2009 for ASEP)

Wedge initial geometry translated to anharmonic chains

Derivative $u = \partial_x h(x,t)$ has a jump for "wedge" initial conditions:



Remember: $\vec{u} = (r, \nu, \mathfrak{e})$ are the local average field variables $\rightsquigarrow$ "domain wall" initial conditions, i.e., solve *Riemann problem*

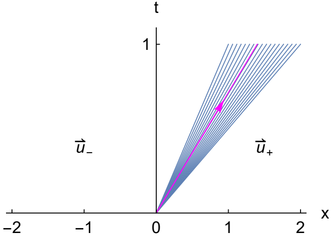
$$\vec{u}(x,0) = \vec{u}_- \quad \text{for} \quad x \leq 0, \qquad \vec{u}(x,0) = \vec{u}_+ \quad \text{for} \quad x > 0$$

Integrated current and TW for anharmonic chains

Integrated current for anharmonic chains (corresponds to $h(x,t)$):

$$\Phi(x,t) = \int_0^t \mathrm{j}(x,t')\,\mathrm{d}t' - \int_0^x u(x',0)\,\mathrm{d}x'$$

(path independent since $(-u, \mathrm{j})$ is curl free)



In analogy to (T)ASEP, for integration within rarefaction wave: expecting

$$\Phi(\mathrm{v}t,t) \simeq a_0 t + (\Gamma t)^{1/3} \xi_{\mathrm{TW}}$$

Linearization of the current for several fields

Explicitly consider *three-component* field $\vec{u}$ (stretch, momentum, energy):

$$A(\vec{u}) = \frac{\partial \mathrm{j}(\vec{u})}{\partial \vec{u}} = \begin{pmatrix} 0 & -\frac{1}{m} & 0 \\ \partial_r P & -\frac{\nu}{m}\partial_e P & \partial_e P \\ \frac{\nu}{m}\partial_r P & \frac{1}{m}P - (\frac{\nu}{m})^2\,\partial_e P & \frac{\nu}{m}\partial_e P \end{pmatrix}$$

with pressure $P(r, e)$

$A(\vec{u})$ has eigenvalues 0 and $\pm c(\vec{u})$, with $c(\vec{u})$ the adiabatic speed of sound:

$$c(\vec{u})^2 = \frac{1}{m}\left(-\partial_r P + P\,\partial_e P\right)$$

Generalization to several fields

Three-component noisy Burgers equation:

$$\partial_t \vec{u} + \partial_x \left(A\vec{u} + \tfrac{1}{2}\langle \vec{u}, \vec{H}\vec{u} \rangle - \partial_x \tilde{D}\vec{u} + \tilde{B}\vec{\xi}(x,t) \right) = 0$$

Hessians: $H^{\alpha}_{\gamma\gamma'} = \partial_{u_\gamma} \partial_{u_{\gamma'}} \mathrm{j}_\alpha, \quad \mathrm{j}_\alpha = \langle \mathcal{J}_\alpha \rangle$

Initial correlations: $\langle u_\alpha(x,0); u_{\alpha'}(x',0) \rangle = C_{\alpha\alpha'}\, \delta(x - x')$

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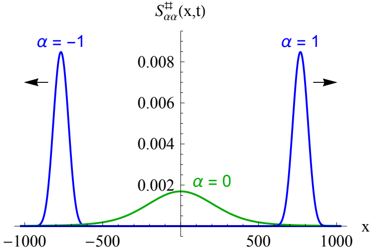
Diagonalization (transformation to normal modes):

$$\vec{\phi} = R\vec{u}, \quad RAR^{-1} = \mathrm{diag}(-c, 0, c), \quad RCR^{\mathrm{T}} = \mathbb{1} \quad \rightsquigarrow$$

$$\partial_t \phi_\alpha + \partial_x\big(c_\alpha \phi_\alpha + \tfrac{1}{2}\langle \vec{\phi}, G^\alpha \vec{\phi}\rangle - \partial_x D\phi_\alpha + B\vec{\xi}(x,t)\big) = 0$$



Riemann problem: Rarefaction curves

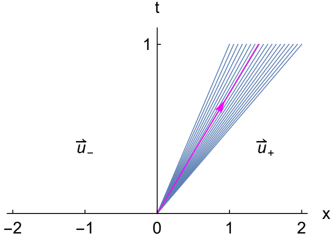
Rarefaction curves: solve the following Cauchy problem in state space (see e.g. Bressan 2013)

$$\partial_\tau \vec{u} = \psi_\alpha(\vec{u}),$$

$\alpha = 0, \pm 1$, where ψ_α are the right eigenvectors of $A = \frac{\partial \mathrm{j}(\vec{u})}{\partial \vec{u}}$.

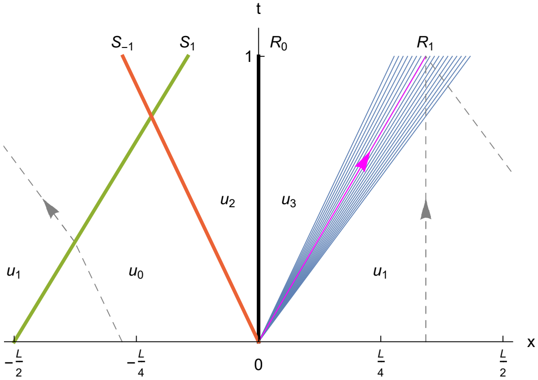
Specifically for eigenvalue σc, $\sigma = \pm 1$:

$$\partial_\tau \begin{pmatrix} r \\ v \\ \mathfrak{e} \end{pmatrix} = \begin{pmatrix} -\frac{1}{m}\sigma \\ c \\ \frac{1}{m}\sigma P + \frac{\nu}{m} c \end{pmatrix}$$



Riemann problem solution for periodic boundaries

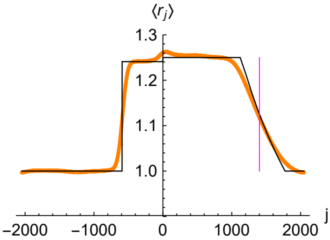
Analytical solution of the *periodic* Riemann problem (anharmonic chain of hard-point particles with alternating masses):

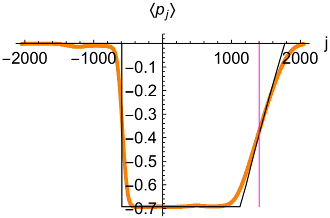


Riemann problem: Molecular dynamics

Average profiles of the stretch $r_j(t)$ and momentum $p_j(t)$ at $t = 1024$

orange dots: molecular dynamics
black curve: analytical solution of the Riemann problem





Transformation to normal modes

Projected current components (with asymptotic value subtracted):

$$\Phi^{\sharp}_{\sigma}(t) = \langle \tilde{\psi}_{\sigma} | \vec{\Phi}(\mathrm{v}t, t) - t(\vec{\mathrm{j}}(\vec{u}_{\mathrm{v}}) - \mathrm{v}\vec{u}_{\mathrm{v}}) \rangle$$

with $\tilde{\psi}_{\sigma}$ the left eigenvectors of $A(\vec{u}_{\mathrm{v}})$
$\Phi^{\sharp}_{1}(t)$ results from perturbations propagating with velocity v along the magenta observation ray $\rightsquigarrow$ expecting

$$\Phi^{\sharp}_{1}(t) \simeq (\Gamma_1 t)^{1/3} \xi_{\mathrm{TW}}$$

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Components $\sigma = -1, 0$ pick up samples from essentially independent space-time regions $\rightsquigarrow$ central limit type behavior

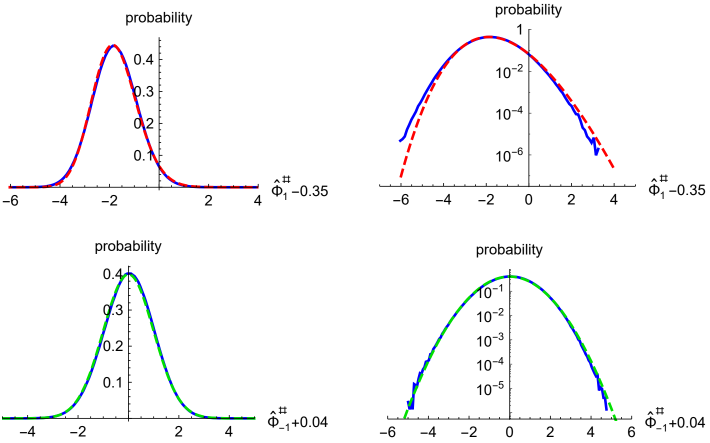
$$\Phi^\sharp_\sigma(t) \simeq (\Gamma_\sigma t)^{1/2} \xi_{\mathrm{G}}, \qquad \sigma = 0, -1,$$

with ξ_{G} a normalized Gaussian random variable

Results based on molecular dynamics simulations

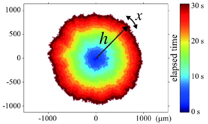
Top row: statistical distribution of $(\Gamma_1 t)^{-1/3}\,\Phi_1^\sharp(t)$

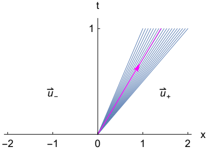
Bottom row: projection $(\Gamma_{-1} t)^{-1/2}\,\Phi_{-1}^\sharp(t)$

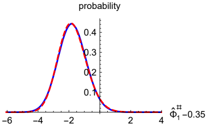


Summary and conclusions

- Nonlinear fluctuating hydrodynamics identified with KPZ equation
- Tracy-Widom GUE distribution emerges for "wedge" initial condition, translates to Riemann problem for anharmonic chains
- Observing Tracy-Widom GUE for projected current component integrated within rarefaction wave







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