Steady velocity of entropic driven interface

- Toward extension to sheared system -

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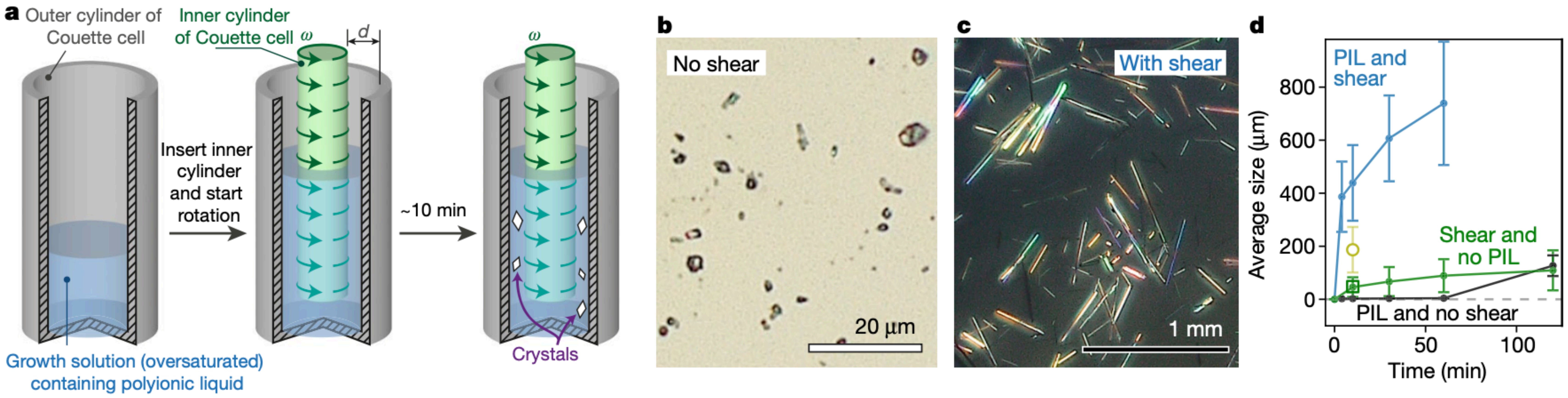
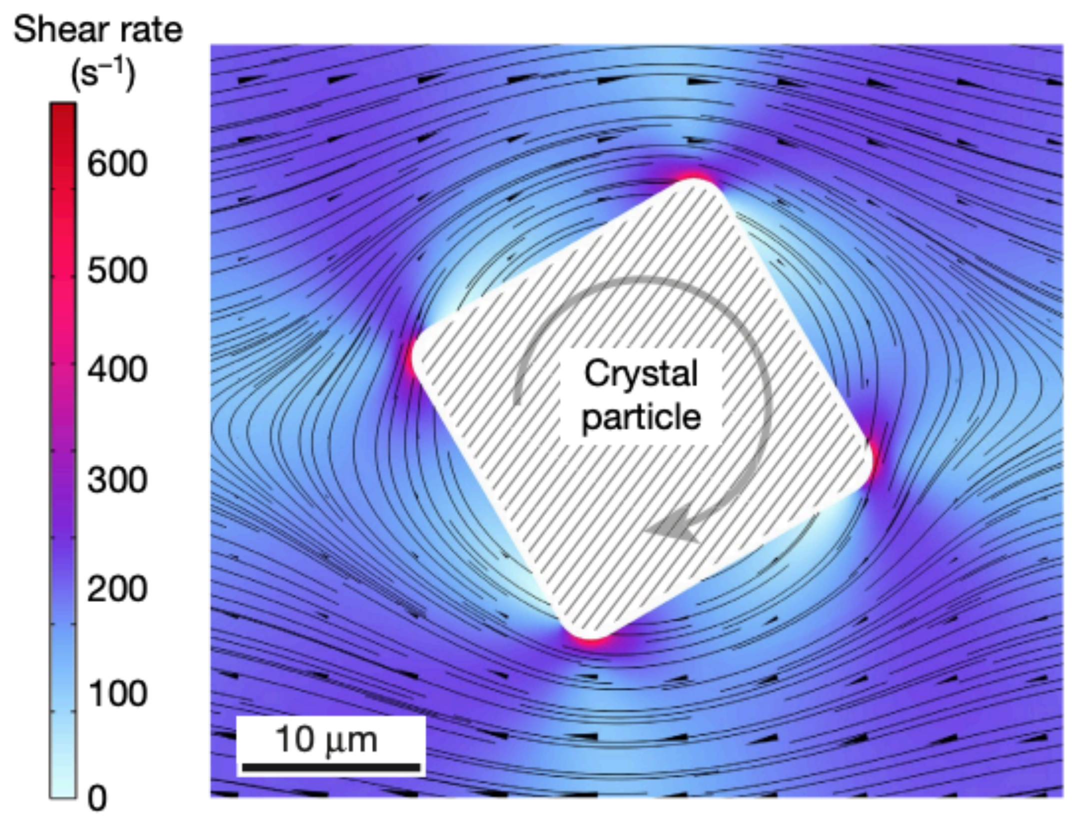
2025 6/6 Hydrodynamics of low-dimensional interacting systems: Advances, challenges, and future directions

Introduction

Motivation : Acceleration of crystal growth by shear flow

Due to presence of polymer and shear flow, melting substance crystalize faster





Salt out caused by polymer

Local shear flow decrease solubility

Jian-Ke Sun et.al Nature, volume 579, pages 73–79 (2020)

→Relation between shear flow and thermodynamic quantities?

Motivation : Theoretical explanation?

- Is the acceleration independent of a specific material?

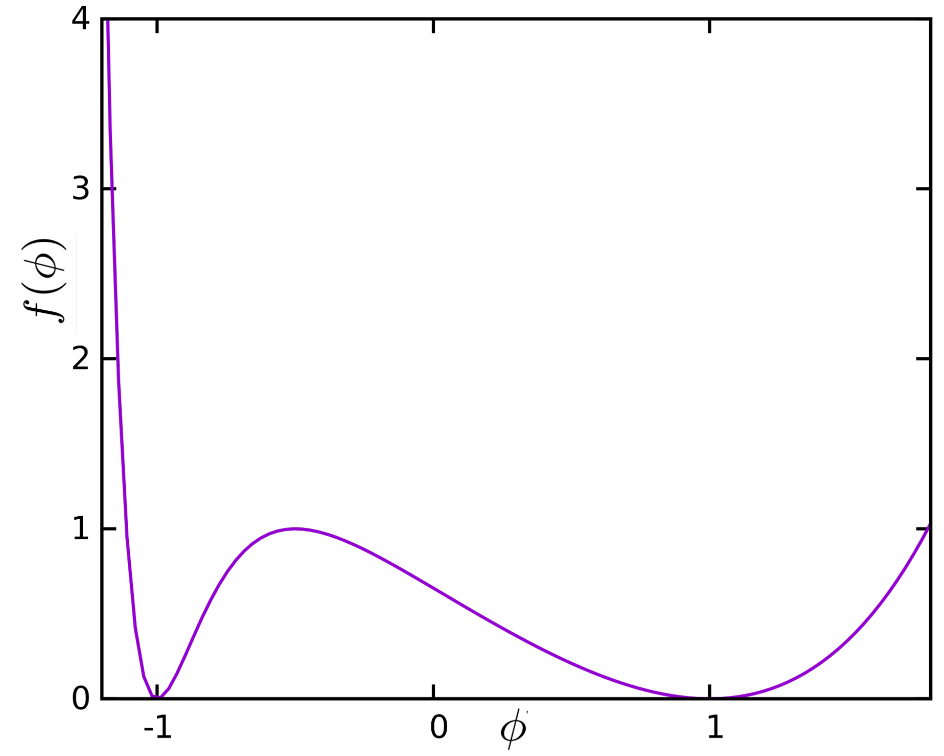
- | Long-range correlation of fluctuations in shear flow systems | + | Entropy force due to fluctuation |

  → A new phenomenon?

→Specific model of an interface driven by entropic forces？

Interface driven by the entropic force

$$\partial_t \phi = -\Gamma[-f'(\phi) - \kappa \partial_x^2 \phi] + \sqrt{2\Gamma T}\eta$$ Hohenberg and Halperin (1977) modelA



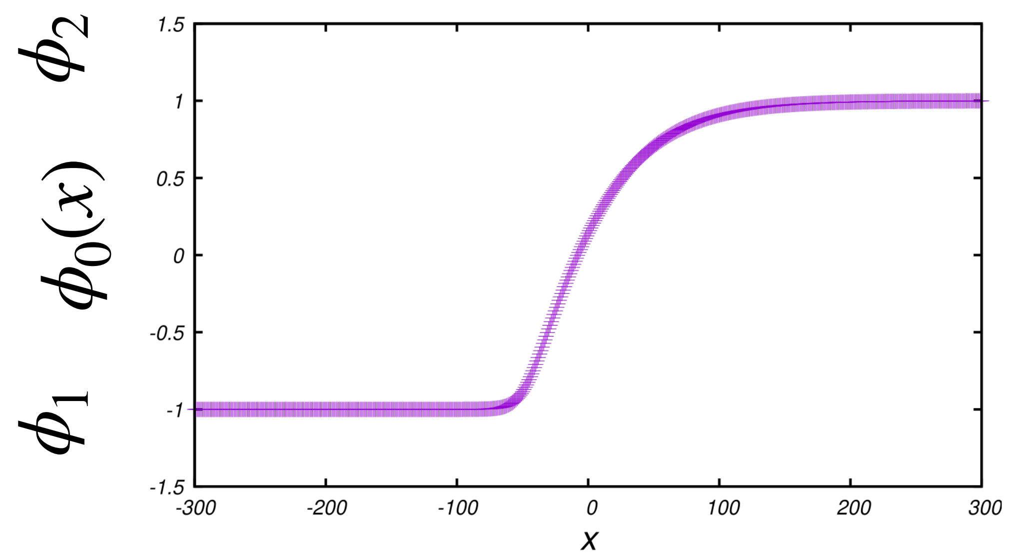
Asymmetric free energy : $f(\phi_1) = f(\phi_2)$, $\underline{f''(\phi_1) \neq f''(\phi_2)}$

$$f(\phi) = \left(\frac{1 - e^{b_1(\phi-1)}}{1 - e^{b_1(\phi_0-1)}} \frac{1 - e^{-b_2(\phi+1)}}{1 - e^{-b_2(\phi_0+1)}} \right)^2$$

$$b_1 = 0.5, b_2 = 5.0, \phi_0 = -0.5$$

Steady solution at $T = 0$: $\phi = \phi_0(x)$

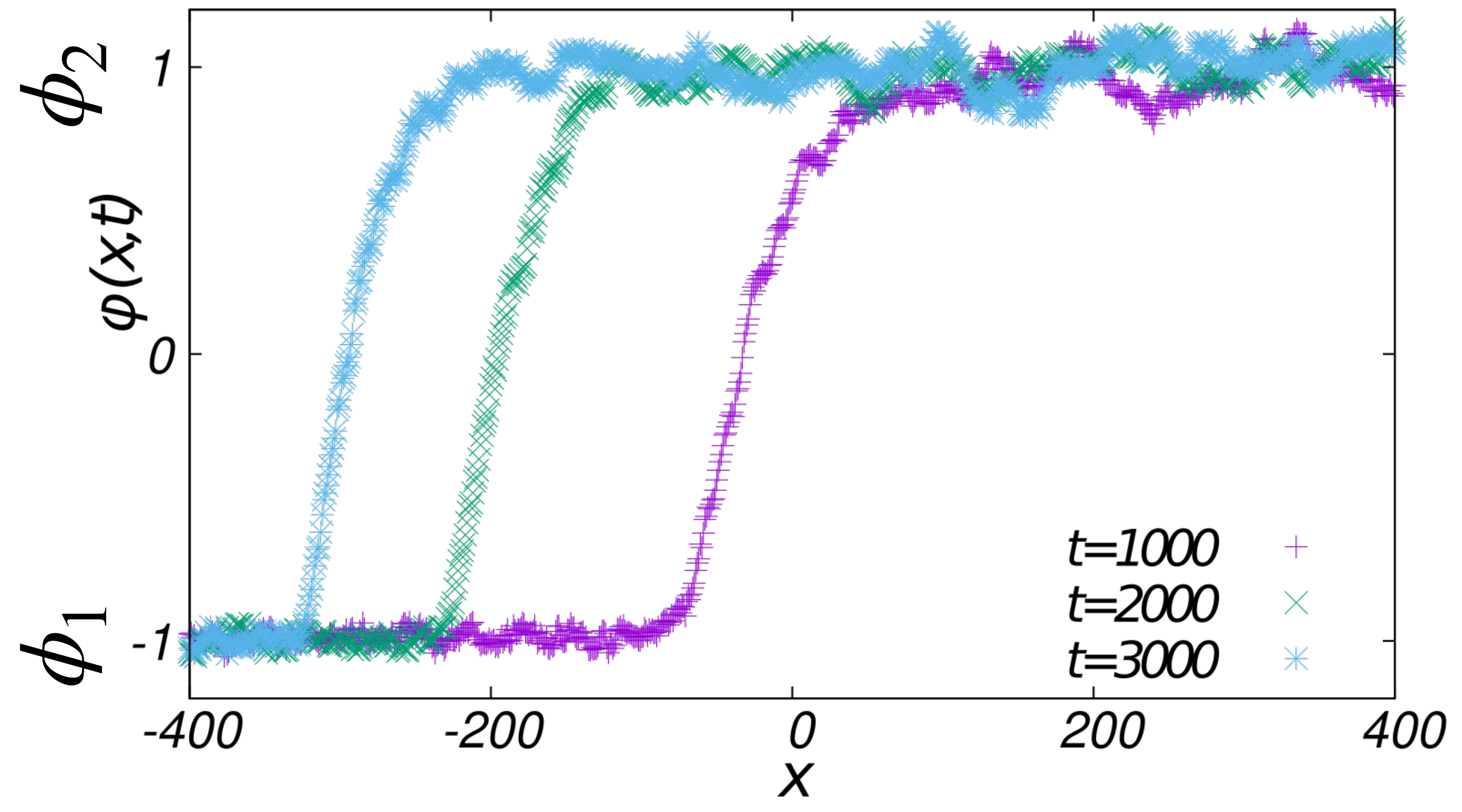
The interface is static. →



In the case $T \neq 0$, fluctuation in bulk regions drives the interface.

Steady velocity: $c = -\frac{\Gamma T(s(\phi_2) - s(\phi_1))}{\int_{-\infty}^{\infty} dz (\partial_z \phi_0(z))^2}$, Entropy density in bulk: $s(\phi_j)$,

When $d = 1$, $s(\phi_2) - s(\phi_1) = -\frac{1}{2}\left(\frac{1}{\xi_2} - \frac{1}{\xi_1}\right)$, Correlation length: $\xi_j = \sqrt{\frac{\kappa}{f''(\phi_j)}}$



Previous research: G. Costantini, et al. PRL, 87, 114102 (2001)

→What non-equilibrium model should be used?

Motivation : The model I want to analyze

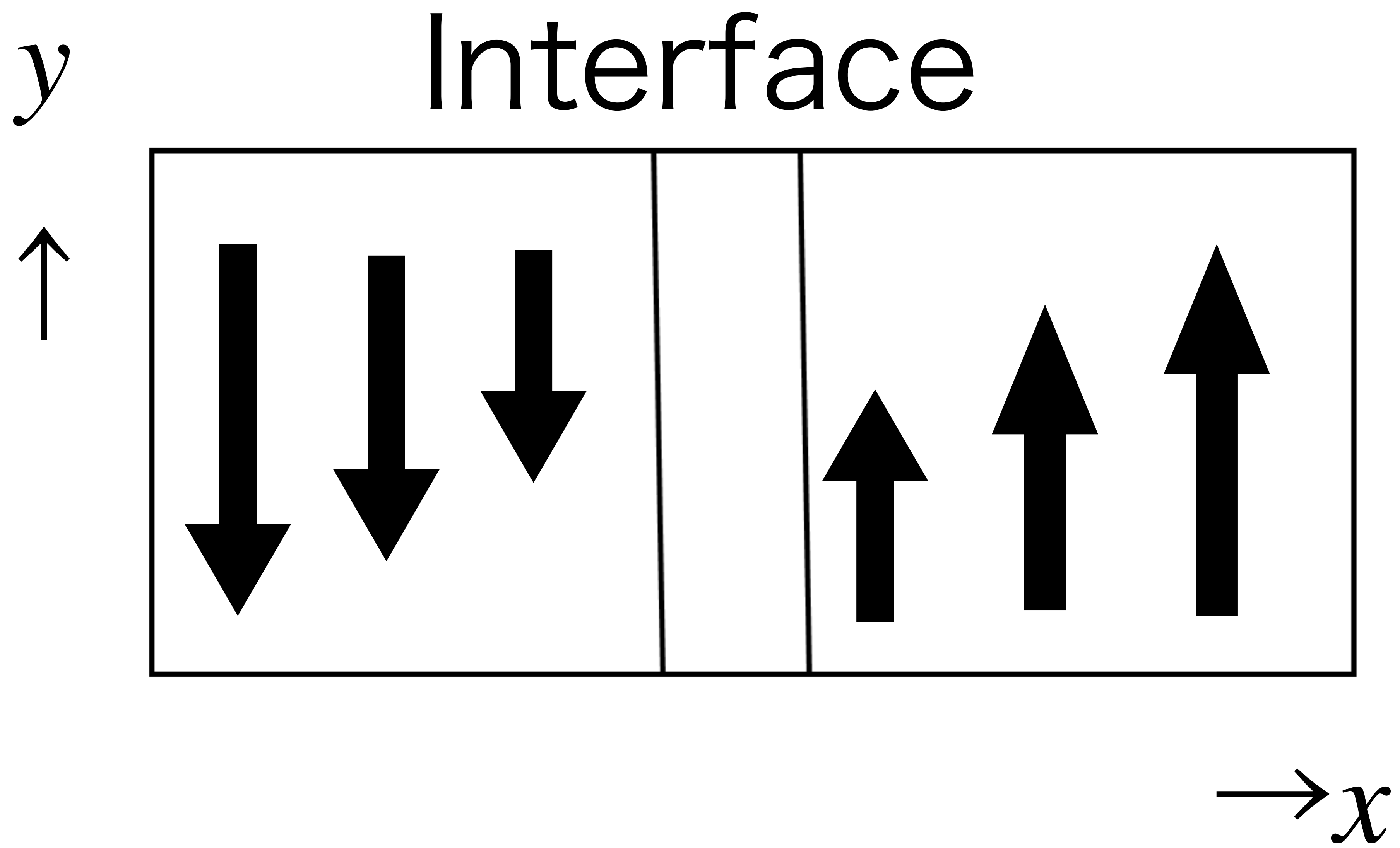
Two dimensional domain : $D \equiv [-\infty, \infty] \times [0, L_y]$

$$(\partial_t + \dot{\gamma} x \partial_y)\phi = -\Gamma[-f'(\phi) - \kappa(\partial_x^2 + \partial_y^2)\phi] + \sqrt{2\Gamma T}\eta$$

Noise: $\langle \eta(\boldsymbol{r}, t)\eta(\boldsymbol{r}', t') \rangle = \delta(\boldsymbol{r} - \boldsymbol{r}')\delta(t - t'), \langle \eta(\boldsymbol{r}, t) \rangle = 0$

Transport coefficient: Γ, Temperature: T, Constant: κ

Velocity of the interface in the x direction?



→How should it be analyzed?

Idea of study

Today's main content

- First, we develop analysis of system without shear flow

  Y. Kado and S.-i. Sasa, Phys. Rev. Lett. 132, 057101(2024)

- Next, we expand the method to shared system (In Progress)

  Explain only steady velocity of interface in sheared system expected in calculations

Analysis of system without shear flow

Reference

Microscopic cut-off dependence of an entropic force in interface propagation of stochastic order parameter dynamics

Y. Kado and S.-i. Sasa, Phys. Rev. Lett. 132, 057101(2024)

Problem

- Develop the analysis of the Interface driven by the entropic force to $d \geq 2$
  c.f. $d = 1$, G. Costantini, et al. PRL, 87, 114102 (2001)

- Calculate the steady velocity of an entropy-driven interface

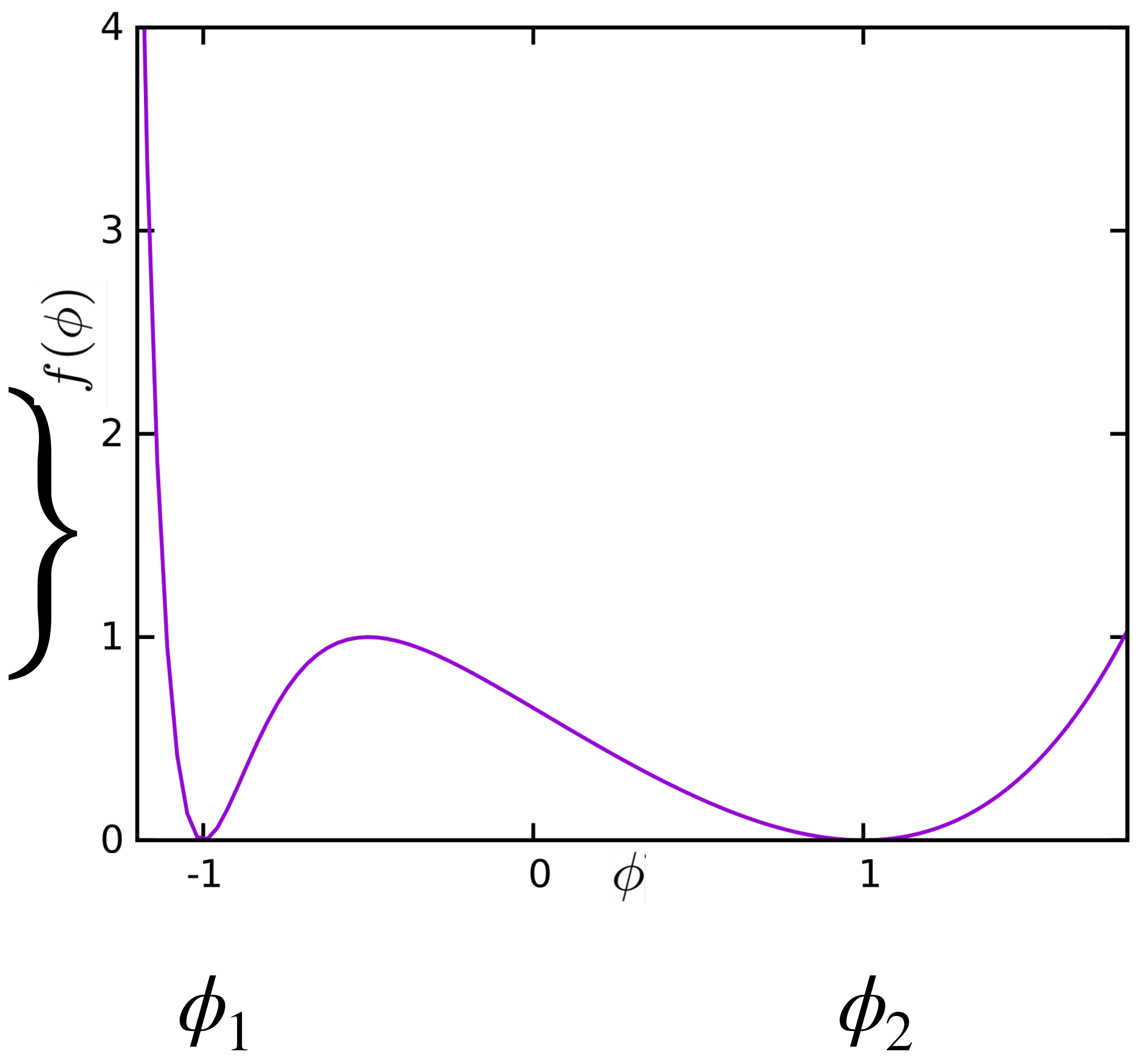
Model (1/2)

Hohenberg and Halperin (1977) modelA

Space region: $D \equiv [-\infty, \infty] \times [0, L_y]$, Order paramter ϕ

Cut-off wave length: k_c i.e. $\phi(\mathbf{k}) = 0 \ (|\mathbf{k}| > k_c)$

Free energy functional: $$\mathscr{F}(\phi) \equiv \int_D d^2\boldsymbol{r} \left\{ f(\phi) + \frac{\kappa}{2}((\partial_x \phi)^2 + (\partial_y \phi)^2) \right\}$$



constant characterizing the interface energy: κ

Free energy density: $f(\phi)$, Two local minima: ϕ_1, ϕ_2

<u>We use asymmetric potential to study driving force by fluctuation</u>

Model (2/2)

Equation of motion: $\partial_t \phi(\mathbf{r}, t) = -\Gamma \frac{\delta \mathcal{F}}{\delta \phi} + \sqrt{2\Gamma T}\eta$

→ $\partial_t \phi = -\Gamma[-f'(\phi) - \kappa(\partial_x^2 + \partial_y^2)\phi] + \sqrt{2\Gamma T}\eta$

Noise: $\langle \eta(\boldsymbol{r}, t)\eta(\boldsymbol{r}', t')\rangle = \delta(\boldsymbol{r} - \boldsymbol{r}')\delta(t - t'), \langle \eta(\boldsymbol{r}, t)\rangle = 0$

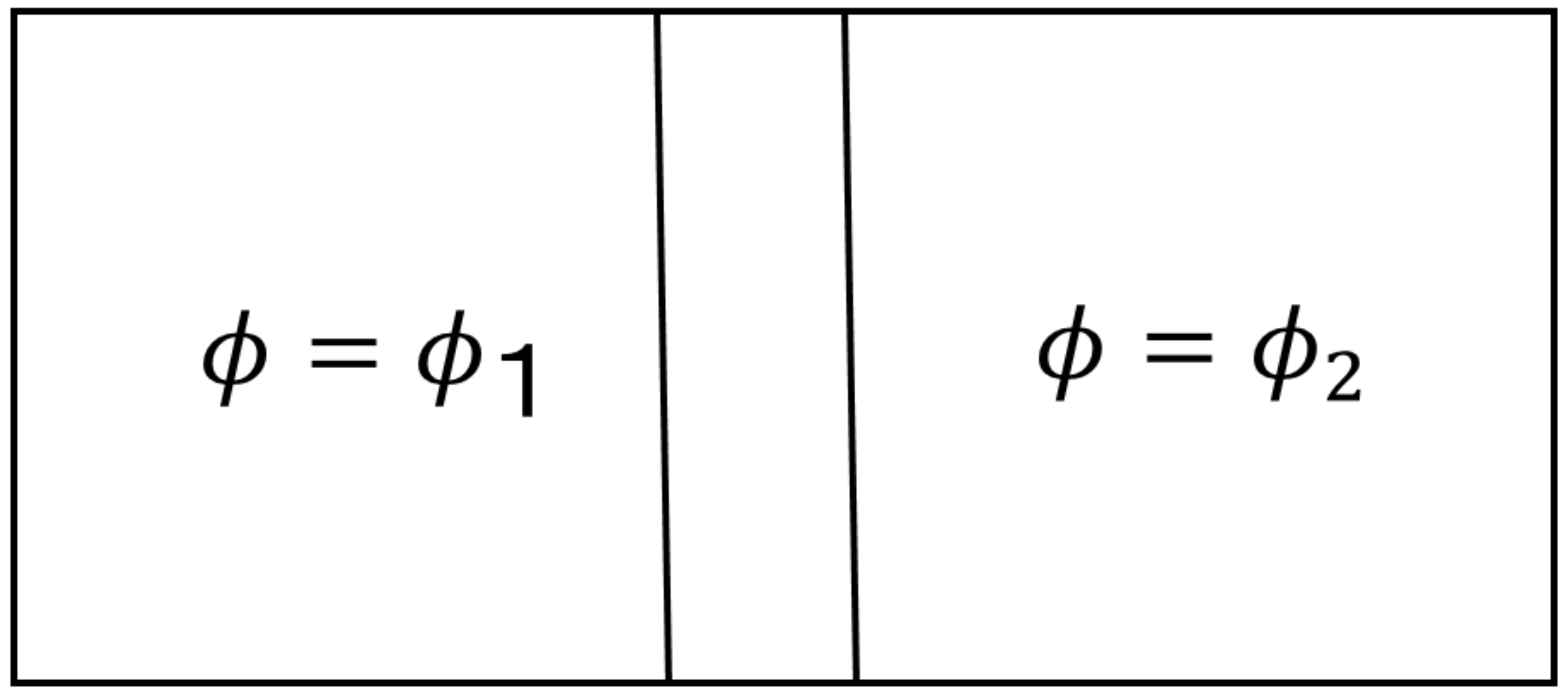
Transport coefficient: Γ, Temperature: T

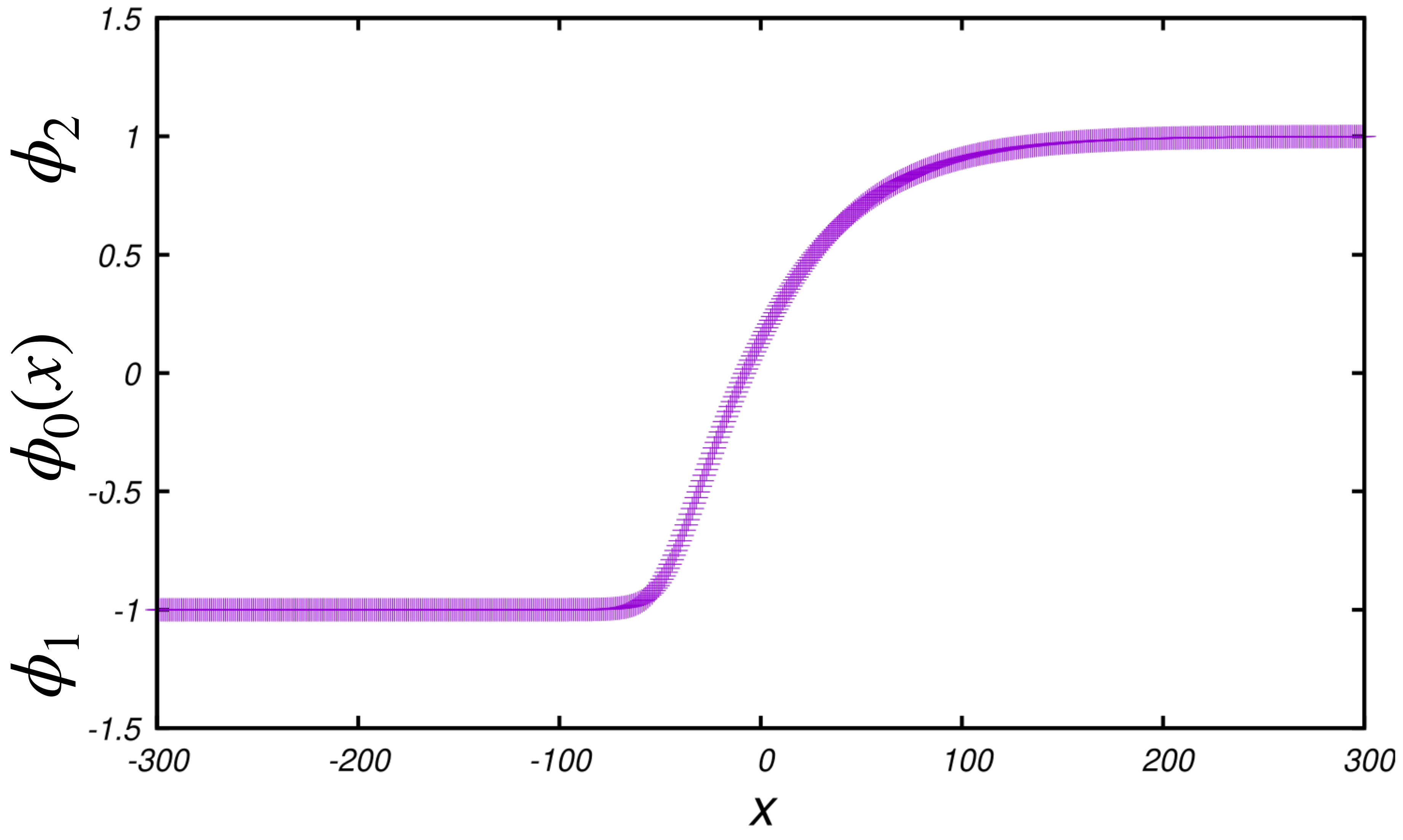
Interface and Boundary condition

x - direction: $\phi(-\infty, y, t) = \phi_1, \phi(\infty, y, t) = \phi_2$

y - direction: Periodic

The interface perpendicular to y - direction





Result : $d = 2$

Result

- steady propagation velocity:

$$c = -\frac{\Gamma T\{s(\phi_2) - s(\phi_1)\}}{\int_{-\infty}^{\infty} dz(\partial_z \phi_0(z))^2}$$

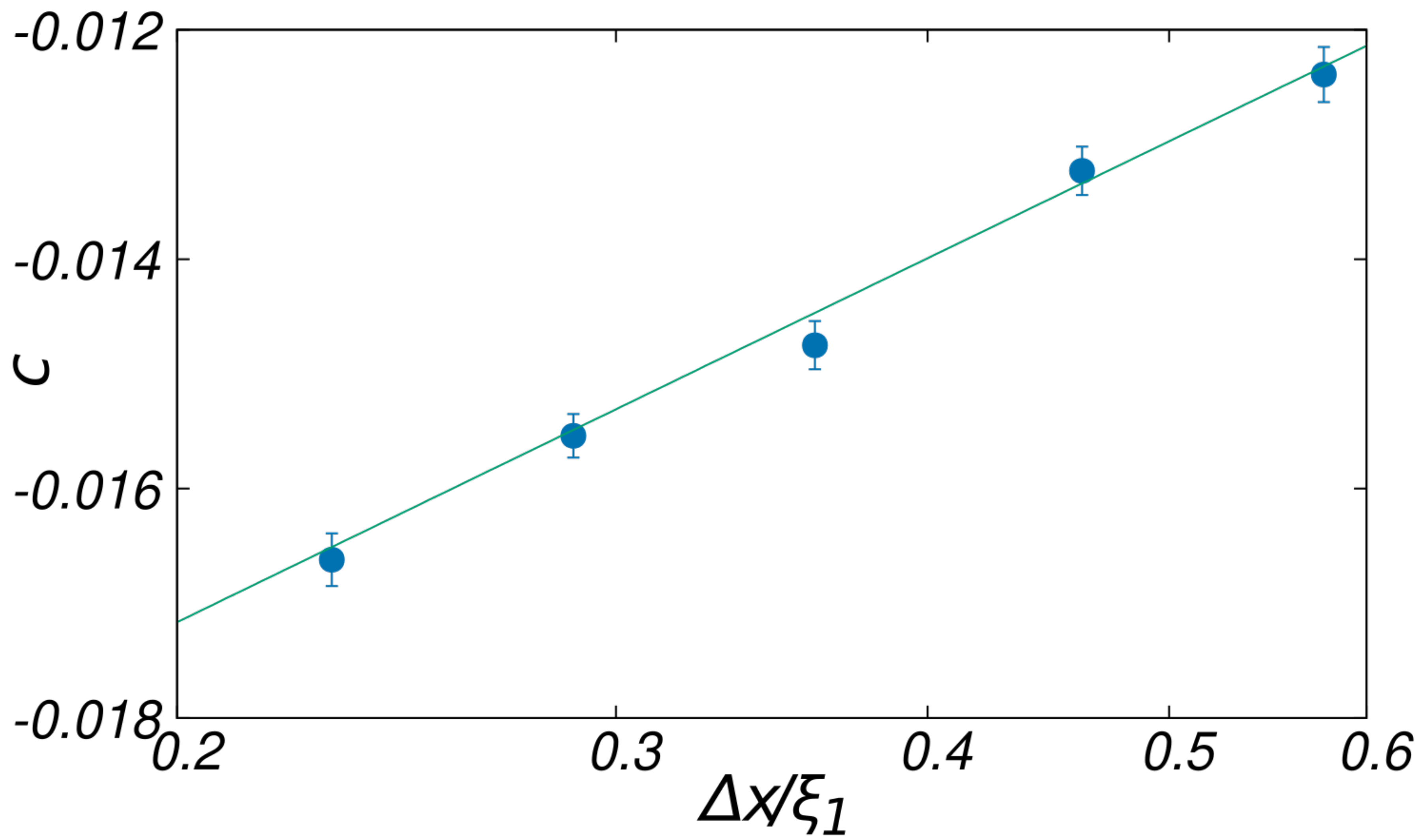
- Entropy density in $d = 2$:

$$s(\phi_j) = -\frac{1}{8\pi\xi_j^2}\ln(\xi_j^2 k_c^2 + 1)$$

- c depends on k_c and,

$|c| \to \infty$ when $k_c \to \infty$

Numerical result



x -direction $[-L, L]$, $L = 400$

$L_y = 100,\ \Delta t = 5.0 \times 10^{-4}\ \Gamma = 0.1,\ T = 0.5,\ \kappa = 1600$

$$k_c = \sqrt{\left(\frac{2\pi}{\Delta x}\right)^2 + \left(\frac{2\pi}{\Delta x}\right)^2} = \frac{2\sqrt{2}\pi}{\Delta x}$$,Δx square lattice size

k_c is corresponding to Δx

Derivation (1/4)

We derive the formula in 2D. $(x, y) \equiv (x_1, x_2)$, $\Gamma \equiv 1$

- Treat the noise as perturbation to stationary solution: ϕ_0
  - Scaling by small dimensionless parameter ϵ : $T = \epsilon^2 T'$, $Y = \epsilon y$
  - co-moving coordinate $z \equiv x - \Theta(Y, t)$, position of interface: $\Theta(Y, t)$
  - Perturbation solution:

$$\phi(x, y, t) = \phi_0(z) + \epsilon \rho_1(z, y, t) + O(\epsilon^2), \qquad \partial_t \Theta = \epsilon \Omega_1([\Theta]) + \epsilon^2 \Omega_2([\Theta]) + O(\epsilon^3)$$

This perturbation method is generalization of
Y. Kuramoto, Prog. Theor. Pays. 63,1885-1903 (1980),
M. Iwata and S.-I., Sasa, PRE 82,11127 (2011).

Derivation (2/4)

We obtain $\partial_t \Theta = \epsilon \Omega_1([\Theta]) + \epsilon^2 \Omega_2([\Theta]) + O(\epsilon^3)$.

$$\Omega_1([\Theta]) = -\frac{\sqrt{2T'}(u_0, \eta)}{(u_0, u_0)},$$

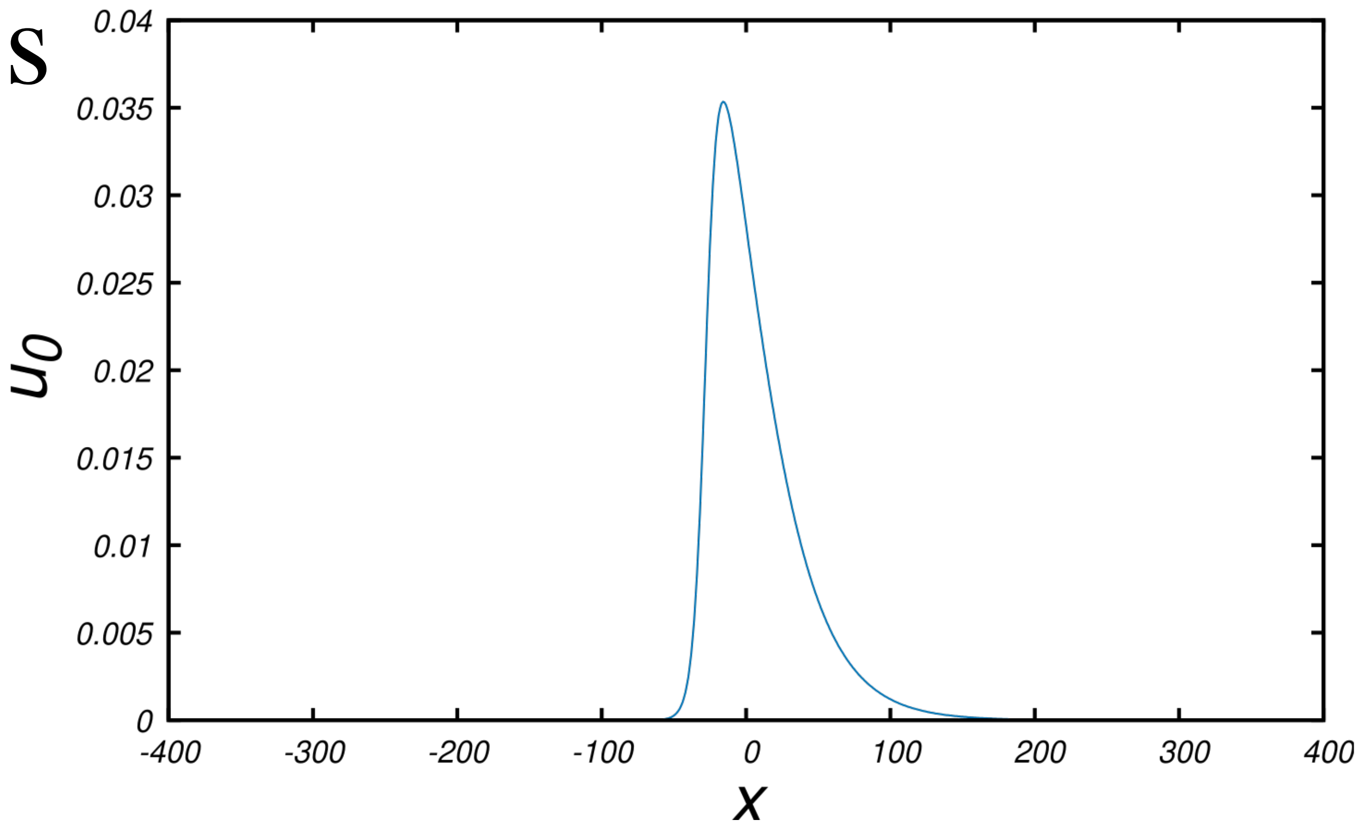
$$(\partial_t - \hat{L}_z - \kappa \partial_y^2)\rho_1(z,t) = \sqrt{2T'}\hat{Q}\eta$$

$$\Omega_2([\Theta]) = \kappa \partial_Y^2 \Theta + \left[\frac{(u_0, \frac{1}{2} f^{(3)}(\phi_0)\rho_1^2)}{(u_0, u_0)} - \Omega_1([\Theta])(u_0, \partial_z \rho_1)\right]$$

- $(a,b) \equiv \frac{1}{L_y}\int_0^{L_y} dy \int_{-\infty}^{\infty} dx a(x,y) b(x,y)$
- Operator: $\hat{L}_z \equiv -f^{(2)}(\phi_0(z)) + \kappa \partial_z^2$, 0 eigen function: $u_0(z) \equiv \partial_z \phi_0(z)$
- Projection: $\hat{Q}a(x) \equiv a(x) - \frac{(u_0, a)}{(u_0, u_0)} u_0(x)$

- Calculate stationary propagation velocity: $c \equiv \langle \partial_t \Theta \rangle_{ss}$

$$\rightarrow \langle \partial_t \Theta \rangle_{ss} = \epsilon^2 \frac{\langle (u_0, \frac{1}{2} f^{(3)}(\phi_0)\rho_1^2)\rangle_{ss}}{(u_0, u_0)} + O(\epsilon^3)$$



Derivation (3/4)

- Express the driving force by **quantities in bulk regions**

$$\langle (u_0, \frac{1}{2} f^{(3)}(\phi_0)\rho_1^2)\rangle_{ss} = \int_{-\infty}^{\infty} dz \frac{1}{2} u_0(z) f^{(3)}(\phi_0(z))\langle \rho_1(z,y)^2\rangle_{ss} = \frac{1}{2}[f^{(2)}(\phi_0)\langle\rho_1^2\rangle_{ss} - \kappa\langle(\partial_z\rho_1)^2\rangle_{ss}]\,|_{z=-\infty}^{z=\infty} + \int_{-\infty}^{\infty} dz \langle \partial_z \rho_1 \hat{L}_z \rho_1\rangle_{ss}$$

$$\int_{-\infty}^{\infty} dz \frac{1}{2}\partial_z\phi_0 f^{(3)}(\phi_0)\rho_1^2 = \int_{-\infty}^{\infty} dz \frac{1}{2}\frac{f^{(2)}(\phi_0(z))}{dz}\rho_1^2$$

$$= \frac{1}{2}[f^{(2)}(\phi_0)\rho_1^2]\,|_{z=-\infty}^{z=\infty} - \int_{-\infty}^{\infty} dz \partial_z\rho_1 f^{(2)}(\phi_0)\rho_1$$

$$= \frac{1}{2}[f^{(2)}(\phi_0)\rho_1^2 - \kappa(\partial_z\rho_1)^2]\,|_{z=-\infty}^{z=\infty} + \int_{-\infty}^{\infty} dz \partial_z\rho_1 \hat{L}_z\rho_1$$

$f''(\phi_0(z)) = -\hat{L}_z + \kappa\partial_z^2$

Use $\int_{-\infty}^{\infty} dz\langle \partial_z\rho_1(z,y,t)\hat{L}_z\rho_1(z,y,t)\rangle_{ss} = \frac{\kappa}{2}\langle(\partial_y\rho_1(z,y,t))^2\rangle_{ss}\,|_{z=-\infty}^{z=\infty}$

Derivation)
- Use time reversal symmetry : $\langle \partial_z\rho_1(z,y,t)\partial_t\rho_1(z,y,t)\rangle_{ss} = 0$
- Multiply $(\partial_t - \hat{L}_z - \kappa\partial_y^2)\rho_1(z,y,t) = \sqrt{2T'}\hat{Q}\eta$ by $\partial_z\rho_1(z,y,t)$, integrate, and calculate expectation

$$= \frac{1}{2} f^{(2)}(\phi_0(\infty))\langle\rho_1(\infty,y)^2\rangle_{ss} - \frac{1}{2} f^{(2)}(\phi_0(-\infty))\langle\rho_1(-\infty,y)^2\rangle_{ss}$$

Derivation (4/4)

- Entropy density： $-Ts(\phi_i) \equiv \frac{1}{2}\epsilon^2 f^{(2)}(\phi_0(\mu_i\infty))\langle\rho_1(\mu_i\infty, y)^2\rangle_{\mathbf{ss}}$

  Here, $\mu_1 = -1,\ \mu_2 = 1$

- Approximate by linearized fluctuation

  $\rightarrow \quad \epsilon^2 f^{(2)}(\phi_0(\mu_i\infty, y))\langle\rho_1(\mu_i\infty, y)^2\rangle_{\mathbf{ss}} = \int_{|\boldsymbol{p}|<k_c} \frac{d\boldsymbol{p}^2}{(2\pi)^2}\frac{T\xi_i^{-2}}{p^2+\xi_i^2} + O(T^{\frac{3}{2}})$

Remark : The case of $d \geq 2$

- When $d \geq 2$, velocity also diverges.

- d-D, $s(\phi_i) = -\frac{1}{2}\int_{|\boldsymbol{p}|\leq k_c} \frac{d^d\boldsymbol{p}}{(2\pi)^d} \frac{\xi_i^2 - p_1^2 + \sum_{l=2}^d p_l^2}{|\boldsymbol{p}|^2 + \xi_i^{-2}}$

  $\rightarrow d = 3$, $s(\phi_i) = \frac{1}{6\pi^2}\left[\frac{k_c}{\xi_i^2} - \frac{1}{\xi_i^3}\tan^{-1}(\xi_i k_c)\right] - \frac{1}{36\pi^2}k_c^2$

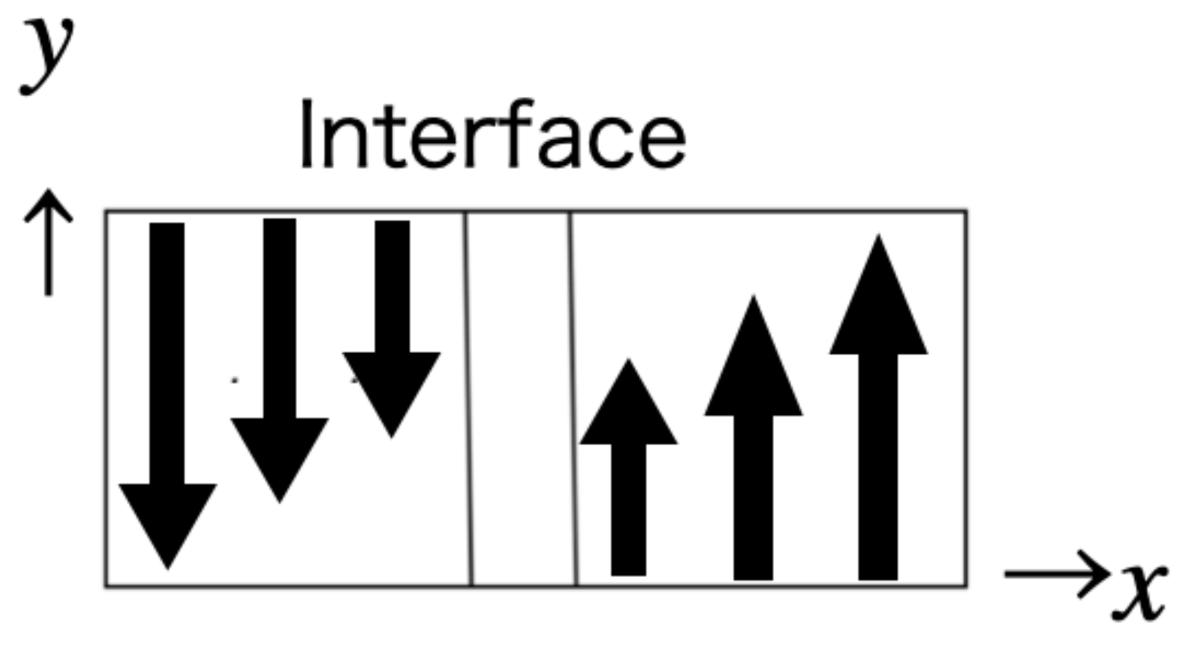
- We calculate the formula in the case $f(\phi_1) = f(\phi_2)$.

  $\rightarrow$ If $f(\phi_1) - f(\phi_2)$ $(\neq 0)$ is small enough, we can treat it as perturbation.

Remark : Steady velocity of sheared system

Calculate velocity of sheared systems as an extension of analysis for equilibrium systems

- Steady velocity of interface : $c = \dfrac{\Gamma\{-T\delta s(\dot{\gamma}) + f_{\rm neq}\}}{\int_{-\infty}^{\infty} dz(\partial_z \phi_0(z))^2}$ → Driving force is decomposed to two ingredient



- Contribution of fluctuation at bulk : $T\delta s(\dot{\gamma}) = Ts(\phi_2;\dot{\gamma}) - Ts(\phi_1;\dot{\gamma})$,

$$-Ts(\phi_i;\dot{\gamma}) = \frac{T}{2}\int_{D_k} \frac{d\mathbf{k}}{(2\pi)^2} \frac{\xi_i^{-2} - k_x^2 + k_y^2}{\xi_i^{-2} + \mathbf{k}^2 + c_0(\Gamma^{-1}\kappa^{-1}|\dot{\gamma}||k_y|)^{2/3}}$$ ←Depend on Cutoff

H. Nakano, Y. Minami, and S.-i. Sasa, Phys. Rev. Lett. 126, 160604 (2021).

- Force caused by time-reversal symmetry breaking : $f_{\rm neq} = \langle(\partial_{x_i}\rho_1, \partial_{t_i}\rho_1 + \dot{\gamma}x_i\partial_{y_i}\rho_1)\rangle_{\rm ss}$

Remark : New nonequilibrium force

- Calculate $f_{\mathrm{neq}} = \langle(\partial_x\rho_1, \partial_t\rho_1 + \dot{\gamma}x\partial_y\rho_1)\rangle_{\mathrm{ss}}$

  Use $\partial_t\rho_1 + \dot{\gamma}x\partial_y\rho_1 = -f^{''}(\phi_0)\rho_1 + \kappa(\partial_x^2 + \partial_y^2)\rho_1 + \sqrt{2T'}\hat{Q}\eta$

  $\rightarrow$ Fourier transformation $\hat{\rho}_1(\mathbf{k}, t) = \int d\mathbf{r}\rho_1(\mathbf{r}, t)e^{i\mathbf{kr}}$ and discretize wave number space

- f_{neq} is non-zero only when $\left(\begin{array}{l} f(\phi) \text{ is asymmetric and} \\ T > 0 \text{ and} \\ \dot{\gamma} \neq 0 \end{array} \right.$

- When $\dot{\gamma}$ is small enough, $f_{\mathrm{neq}} = TB\dot{\gamma} + TC\dot{\gamma}^2 + O(\dot{\gamma}^3)$, B, C : constants

Remark : Future task

- Numerical calculation of velocity of interface in sheared media

- $T\delta s(\dot{\gamma})$ and f_{neq} 's dependency of $\dot{\gamma}$?

- Velocity of interface increase or decrease?

Conclusion

- We developed analysis of entropic driven interface.

- Due to time reversal symmetry of equilibrium system, we showed driving force of interface is given by the difference of fluctuations at bulk.

  →In sheared system, modified entropic force and force caused by time reversal symmetry breaking may appear?

- Steady velocity of interface driven by entropic force in $d \geq 2$

  - Cut-off dependence: $k_c \to \infty$, $|c| \to \infty$

  - in numerical simulations, k_c is Wavenumber corresponding to mesh size Δx

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Derivation : Perturbation

Co-moving with interface and flow : $x_f = x - \Theta(Y,t), y_f = y - \dot{\gamma}xt, t_f = t$

Perturbation expansion :$Y = \epsilon y, T = \epsilon^2 T'$ $\quad (f,g) \equiv \frac{1}{L_y}\int_D dxdyf(x,y)g(x,y)$, $u_0(x) = \partial_x \phi_0(x)$

$$\phi(x,y,t) = \phi_0(x_f) + \epsilon\rho_1(x_f, y_f, t_f) + O(\epsilon^2)$$
$$\partial_t \Theta = \epsilon\Omega_1([\Theta]) + \epsilon^2\Omega_2([\Theta]) + O(\epsilon^3)$$

$$O(\epsilon): \ \partial_{t_f}\rho_1 = -f''(\phi_0)\rho_1 + \kappa((\partial_{x_f} - \dot{\gamma}t\partial_{y_f})^2 + \partial_{y_f}^2)\rho_1 + \sqrt{2T'}\hat{Q}\eta,\ \Omega_1([\Theta]) = -\frac{\sqrt{2T'}(u_0,\eta)}{(u_0,u_0)}$$

$$O(\epsilon^2): -\Omega_2(u_0,u_0) - \partial_Y\Theta[\dot{\gamma}\Theta(u_0, x_f\partial_{x_f}\rho_1) + \dot{\gamma}(u_0, x_f\partial_{x_f}\rho_1)] = -\frac{1}{2}(u_0, f^{(2)}(\phi_0)\rho_1^2) - \kappa\partial_Y^2\Theta(u_0,u_0) + g(\phi_2 - \phi_1)$$

Result :$\left\langle \frac{1}{\epsilon L_y}\int dY\Omega_2 \right\rangle_{\rm ss}(u_0,u_0) = \frac{1}{2}\langle (u_0, f^{(2)}(\phi_0)\rho_1^2)\rangle_{\rm ss}$

Derivation : decompose of driving force

Co-moving with interface : $x_i = x_f, y_i = y_f + \dot{\gamma} x t, t_i = t_f$

$$\rho_1(\mathbf{r_f}, t_f) = \rho_1(\mathbf{r_i}, t_i), \quad \partial_{t_i}\rho_1 + \dot{\gamma} x_i \partial_{y_i}\rho_1 = -f^{''}(\phi_0)\rho_1 + \kappa(\partial_{x_i}^2 + \partial_{y_i}^2)\rho_1 + \sqrt{2T'}\hat{Q}\eta$$

$$\frac{1}{2}\langle (u_0, f^{(2)}(\phi_0)\rho_1^2)\rangle_{\rm ss} = \langle \Psi(x_i)\rangle_{\rm ss}|_{x_i=-\infty}^{x_i=\infty} + \langle (\partial_{t_i}\rho_1, \partial_{t_i}\rho_1 + \dot{\gamma} x_i \partial_{y_i}\rho_1)\rangle_{\rm ss} + \langle (\partial_{x_i}\rho_1, \sqrt{2T'}\hat{Q}\eta)\rangle_{\rm ss}$$

$$\Psi(x_i, y_i, t) \equiv \frac{1}{2}[f^{(2)}(\phi_0)\rho_1^2 - \kappa(\partial_{x_i}\rho_1)^2 + \kappa(\partial_{y_i}\rho_1)^2]$$

Entropic force by fluctuation at bulk : $-Ts(\phi_i; \dot{\gamma}) = \frac{T}{2}\int_{D_k} \frac{d\mathbf{k}}{(2\pi)^2} \frac{\xi_i^{-2} - k_x^2 + k_y^2}{\xi_i^{-2} + \mathbf{k}^2 + c_0(\Gamma^{-1}\kappa^{-1}|\dot{\gamma}||k_y|)^{2/3}},$

Contribution at interface region : $f_{\rm neq} = \langle (\partial_{t_i}\rho_1, \partial_{t_i}\rho_1 + \dot{\gamma} x_i \partial_{y_i}\rho_1)\rangle_{\rm ss}$

Derivation : Calculation of $f_{\rm neq}$

$$f_{\rm neq} = \langle (\partial_{t_i}\rho_1, \partial_{t_i}\rho_1 + \dot{\gamma} x_i \partial_{y_i}\rho_1) \rangle_{\rm ss},$$

$\partial_{t_i}\rho_1 + \dot{\gamma} x_i \partial_{y_i}\rho_1 = -f^{''}(\phi_0)\rho_1 + \kappa(\partial_{x_i}^2 + \partial_{y_i}^2)\rho_1 + \sqrt{2T'}\hat{Q}\eta$ → Fourier transformation $\hat{\rho}_1(\mathbf{k}, t) = \int d\mathbf{r}\rho_1(\mathbf{r}, t)e^{i\mathbf{kr}}$

$\partial_t \hat{\rho}_1(\mathbf{k}) - \dot{\gamma} k_y \partial_{k_x}\hat{\rho}_1 = -\int \frac{dk_x'}{(2\pi)} \hat{f}^{(2)}(k_x - k_x')\hat{\rho}_1(k_x', k_y) - \kappa(k_x^2 + k_y^2)\hat{\rho}_1(k_x, k_y) + \hat{\eta}$ → discretize k_x, k_y

$$\partial_t \hat{\rho}_1(\mathbf{k}) - \dot{\gamma} k_y \partial_{k_x}\hat{\rho}_1 = -\sum_{k_x'} M(k_x, k_x'; k_y)\hat{\rho}(k_x', k_y) + \hat{\eta}(k_x, t),\ M(k_x, k_x'; k_y) = \frac{1}{2\pi}\hat{f}^{(2)}(k_x - k_x')\Delta k + \kappa(k_x^2 + k_y^2)\delta_{k_x, k_x'}$$

$$f_{\rm neq} \simeq -(2\pi)^2 2T\kappa \sum_{\mathbf{k}} ik_x \int_{-\infty}^{0} ds(2k_x\dot{\gamma}k_y s + \dot{\gamma}^2 k_y^2 s^2)\exp(2L(s; k_y, \dot{\gamma}))_{k_x, k_x},\ L_{k_x, k_x'}(s; k_y, \dot{\gamma}) = \int_0^s ds' M(k_x(s'), k_x'(s'); k_y),\ k_x(s) = k_x - \dot{\gamma}k_y s$$

→ If $\dot{\gamma} = 0$ (equilibrium) or potential $f(\phi)$ is symmetric, $f_1 = 0$

When $\dot{\gamma}$ is small enough, $f_{\rm neq} = TB\dot{\gamma} + O(\dot{\gamma}^2),\ B = -\dot{\gamma}(2\pi)^2 4\kappa \sum_{\mathbf{k}} ik_x^2 k_y \int_{-\infty}^{0} dss\exp(2L(s; k_y, \dot{\gamma} = 0))_{k_x, k_x}$