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

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Background: Description of phenomena

- Existence of deterministic equations: Macroscopic fluid

- Absence of deterministic equations:

Order parameter near a critical point

Hohenberg and Halperin, Rev. Mod. Phys. 49, 435 (1977)

Locally conserved quantities in one or two dimensions

D. Forster, D. R. Nelson, and M. J. Stephen, Phys. Rev. A 16, 732 (1977)

Background: Infrared divergence

Fluctuating hydrodynamic equation

→ Infrared divergence of Renormalized transportation coefficients in 1D and 2D

→Deterministic hydrodynamic equation **CANNOT** describe 1D and 2D Fluid.

→Violation of scale separation between macro and meso

Purpose and Result

Another violation of scale separation?

Result:

Propagation velocity of a planer interface in $d \geq 2$

by stochastic order parameter dynamics

→Dependence on the microscopic **ultraviolet cut-off**

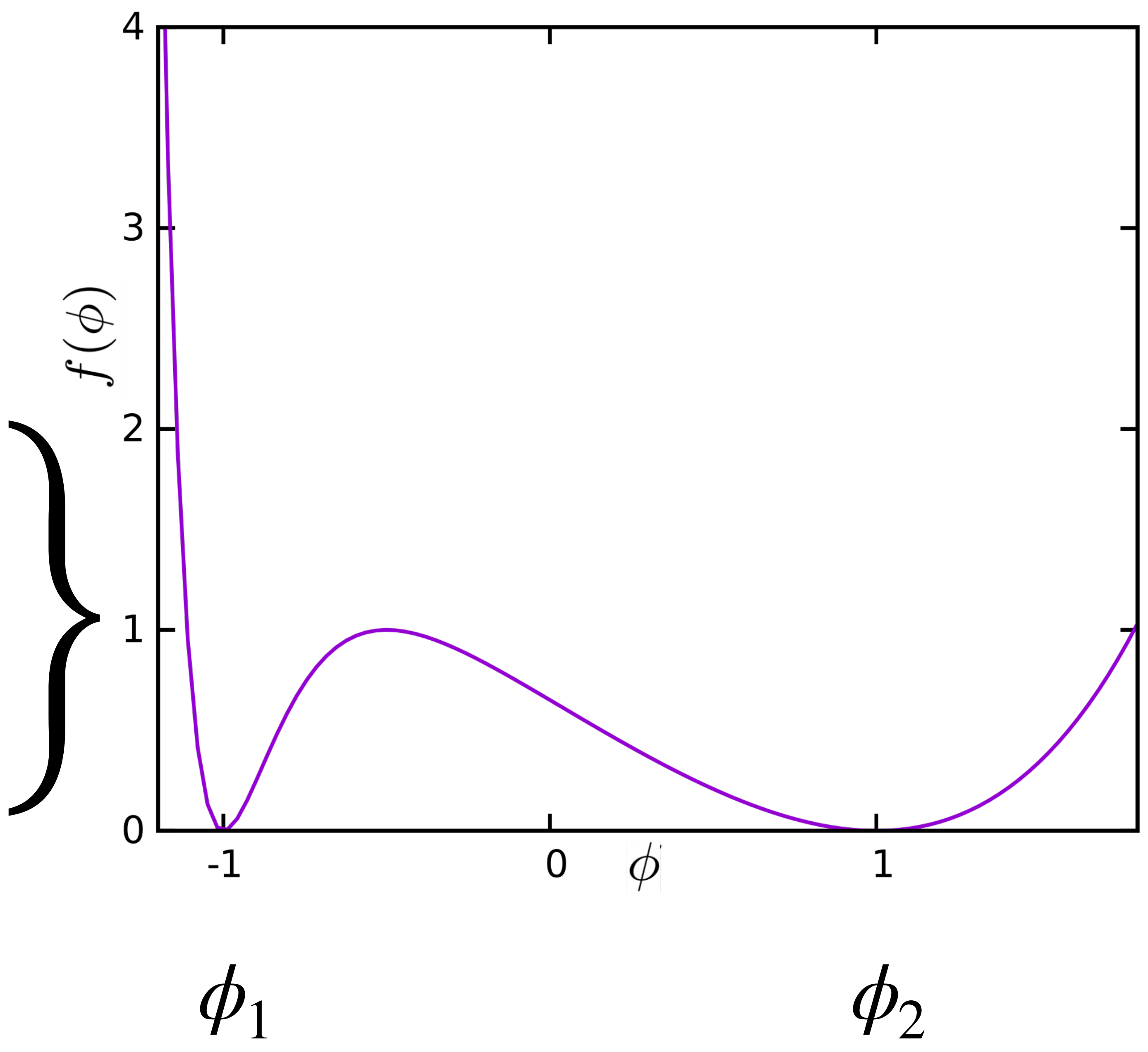
Model (1/2)

Hohenberg and Halperin (1977) modelA

Space region: $D \equiv [-\infty, \infty] \times [0, L_y]^{(d-1)}$, Order paramter ϕ

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

Free energy functional: $\mathscr{F}(\phi) \equiv \int_D d^d\boldsymbol{r} \left\{ f(\phi) + \frac{\kappa}{2} \sum_{i=1}^{d} (\partial_{x_i}\phi)^2 \right\}$



constant characterizing the interface energy: κ

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

Model (2/2)

Equation of motion: $\partial_t \phi = -\Gamma \frac{\delta \mathscr{F}}{\delta \phi} + \sqrt{2\Gamma T}\eta$

→ $$\partial_t \phi = -\Gamma[-f'(\phi) - \kappa \sum_{i=1}^{d} (\partial_{x_i}\phi)^2] + \sqrt{2\Gamma T}\eta$$

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

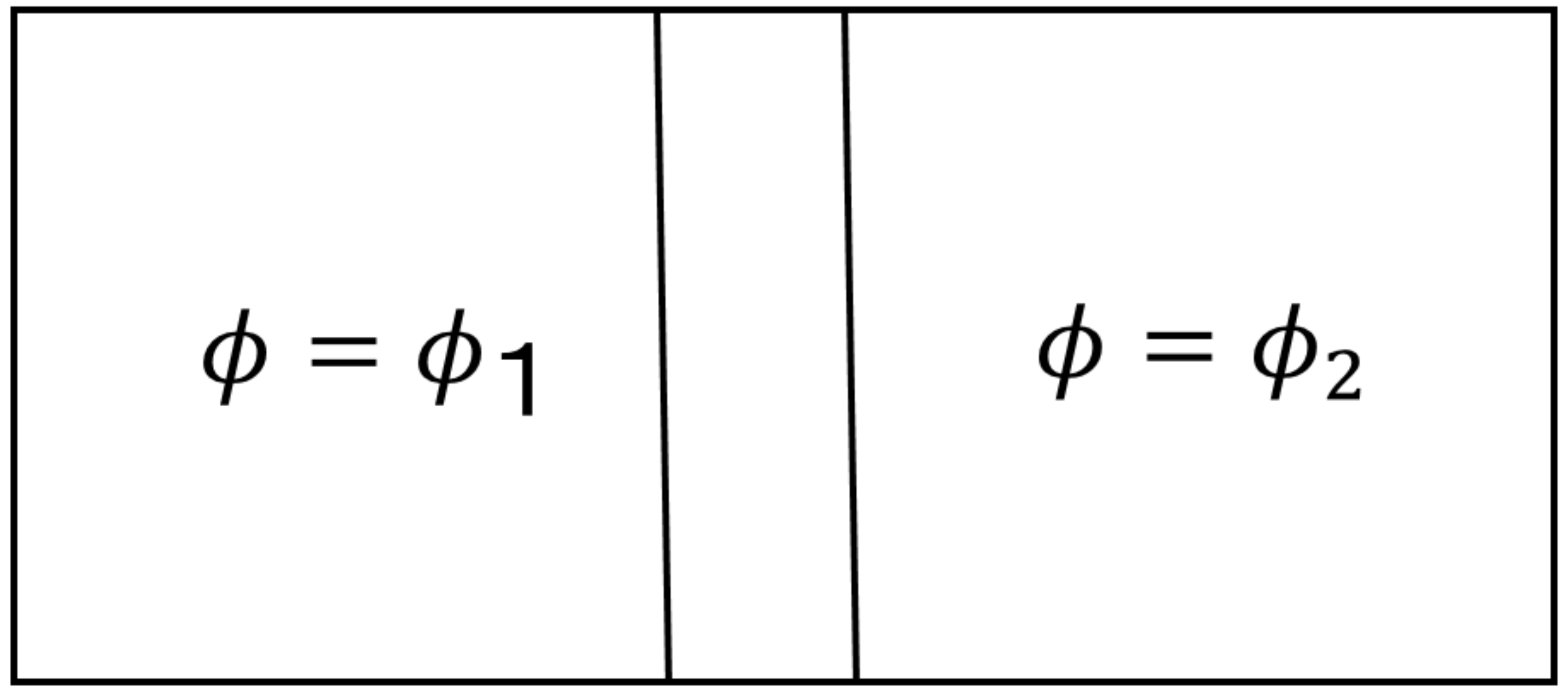
Transport coefficient: Γ, Temperature: T

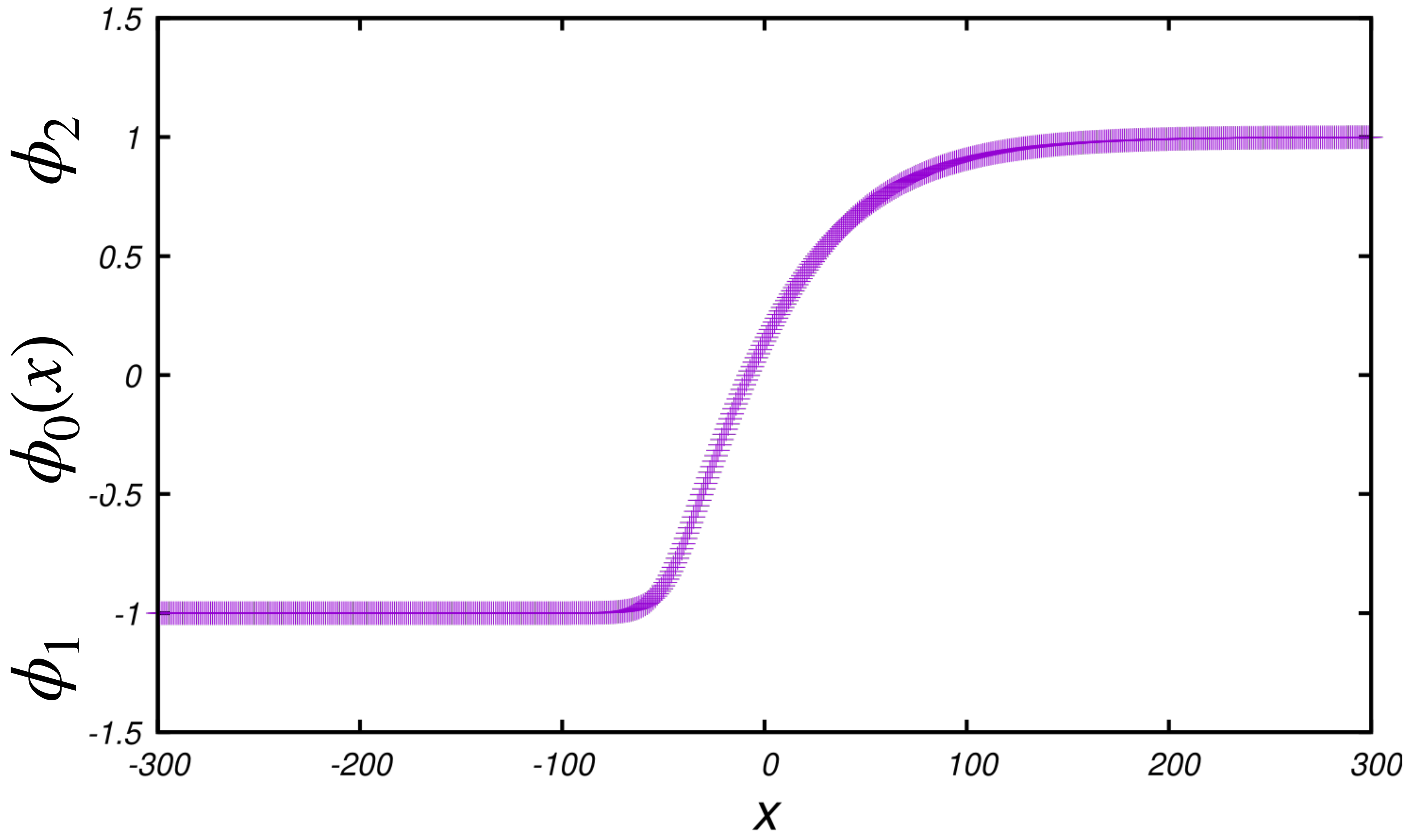
Interface and Boundary condition

$x_1(=x)$ - direction: $\phi(-\infty, x_2, \cdots, x_d, t) = \phi_1, \phi(\infty, x_2, \cdots, x_d, t) = \phi_2$

$x_2, \cdots, x_d$ - direction: Periodic

The interface perpendicular to x_1 - direction





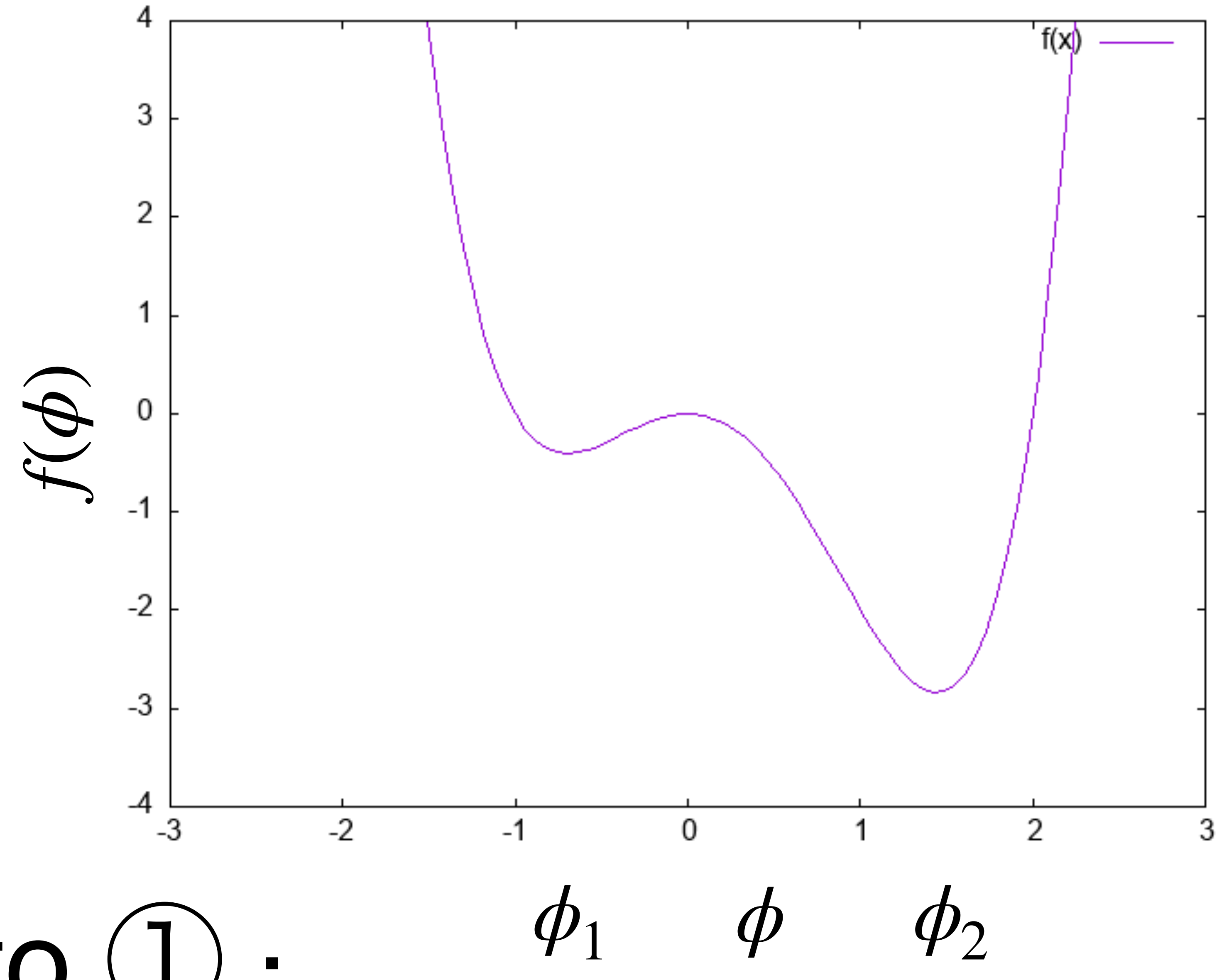
The case T=0 : Trivial case

$$\partial_t \phi = -\Gamma[f'(\phi) - \kappa \partial_x^2 \phi] \quad \text{—①}$$

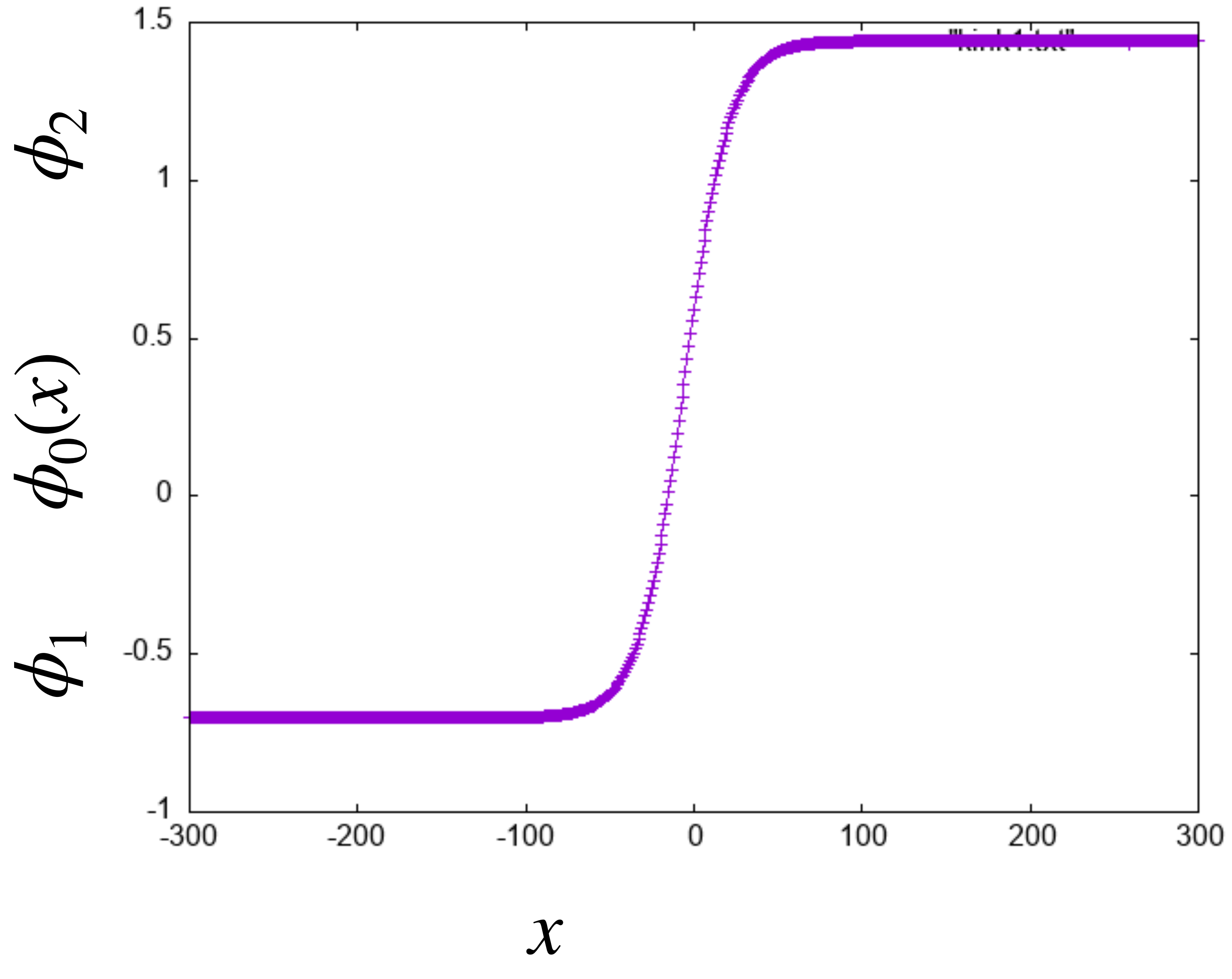
Substitute $\phi(x, x_2, \cdots, x_d, t) = \phi_0(z), z \equiv x - c_0 t$ to ① :

$$-c_0 \partial_z \phi_0 = -\Gamma[f'(\phi_0) - \kappa \partial_z^2 \phi_0]$$

Propagation velocity: $c_0 = \dfrac{\Gamma(f(\phi_2) - f(\phi_1))}{\int_{-\infty}^{\infty} dz (\partial_z \phi_0(z))^2}$



$f(\phi) = \phi^4 - \phi^3 - 2\phi^2$

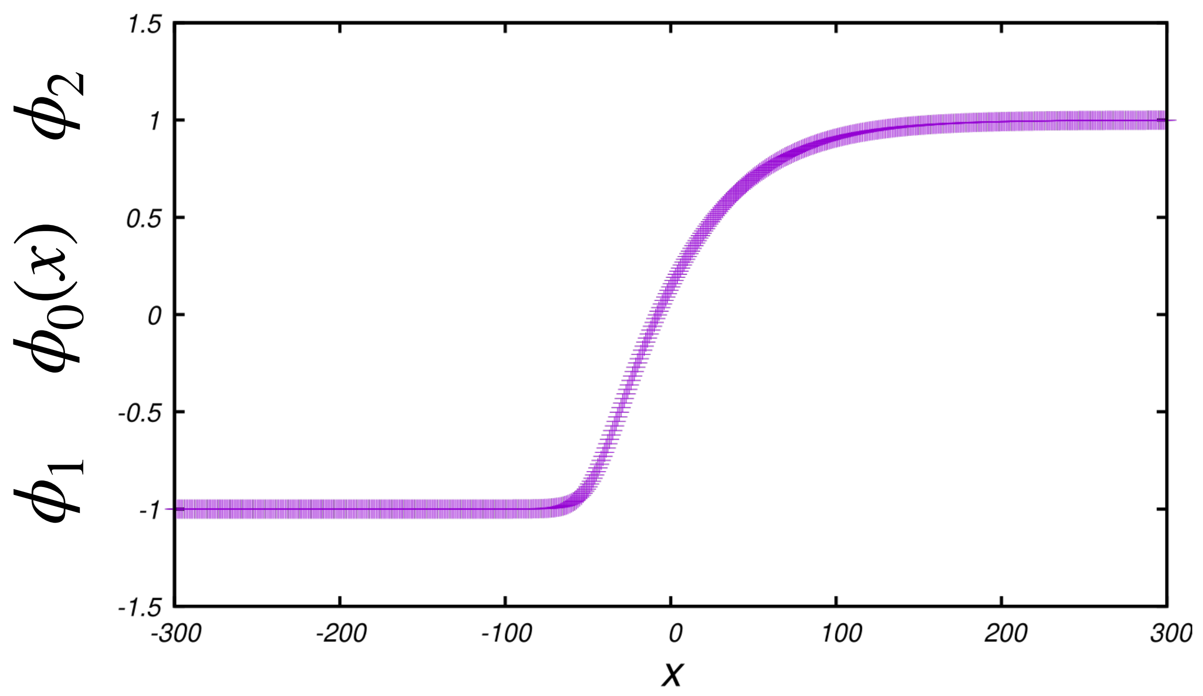


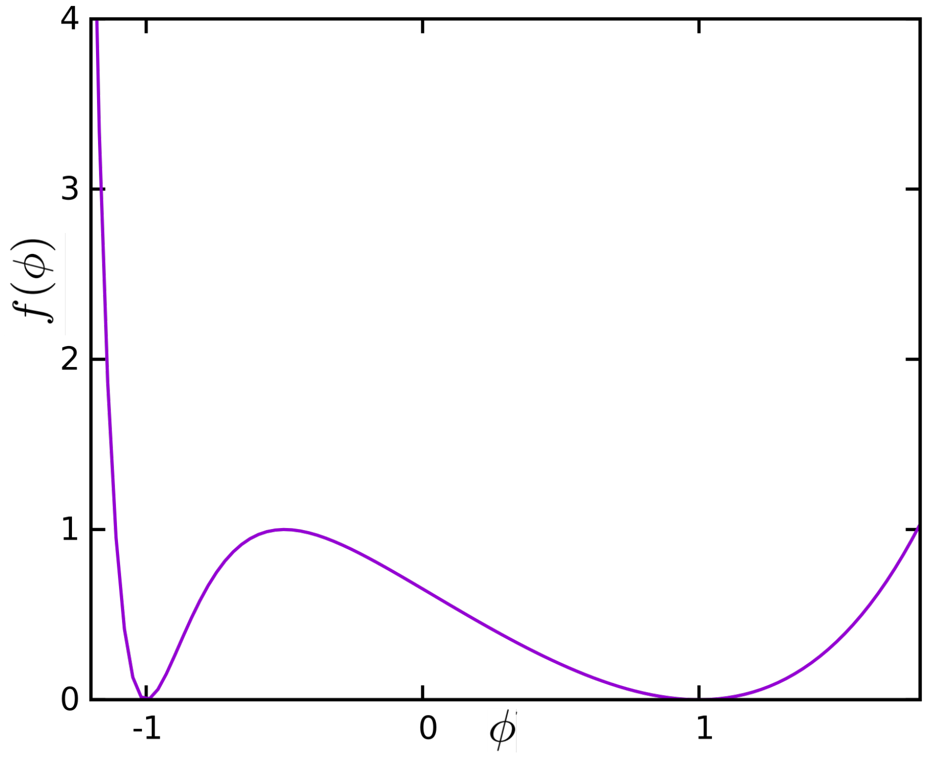
The case $T \neq 0$: Interface driven by the entropic force

$f(\phi_1) = f(\phi_2)$, $f''(\phi_1) \neq f''(\phi_2)$

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

The interface is static. →





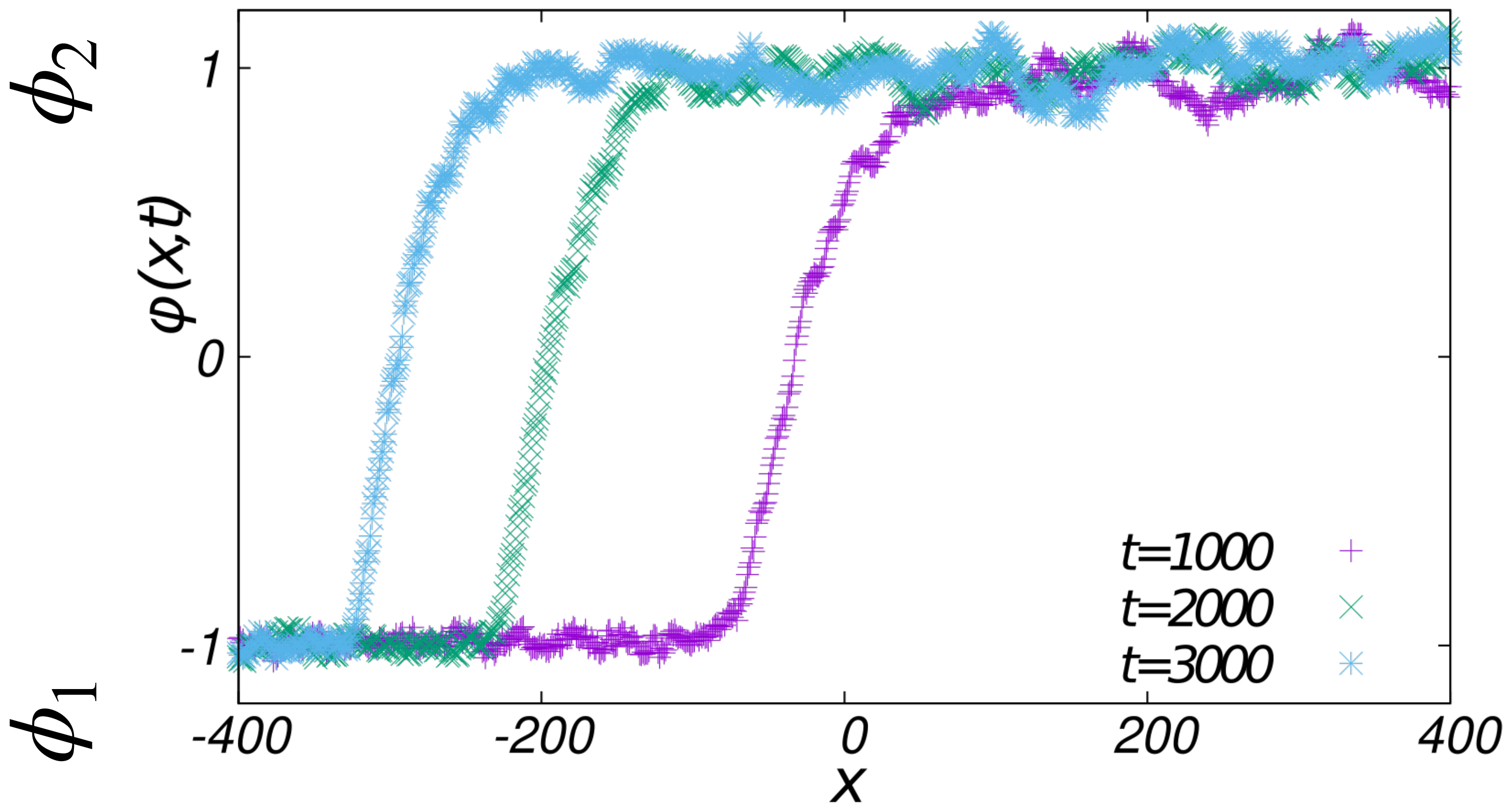
$$f(\phi) = \left(\frac{1 - e^{b_1(\phi - 1)}}{1 - e^{b_1(\phi_0 - 1)}} \frac{1 - e^{-b_2(\phi + 1)}}{1 - e^{-b_2(\phi_0 + 1)}} \right)^2$$

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

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

Steady velocity: $c = -\dfrac{\Gamma T(s(\phi_2) - s(\phi_1))}{\int_{-\infty}^{\infty} dz (\partial_z \phi_0(z))^2}$,

Entropy density in bulk: $s(\phi_j)$,



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

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

Problem

Steady propagation velocity of a $(d-1)$-D planer interface d-D

- Derivation in d -D

  $\rightarrow$ Previous research：Not applicable

  $\rightarrow$ New method

- Numerical simulation when $d = 2$

  $\rightarrow$ No research

Result : $d = 2$

Result

・ steady propagation velocity:

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

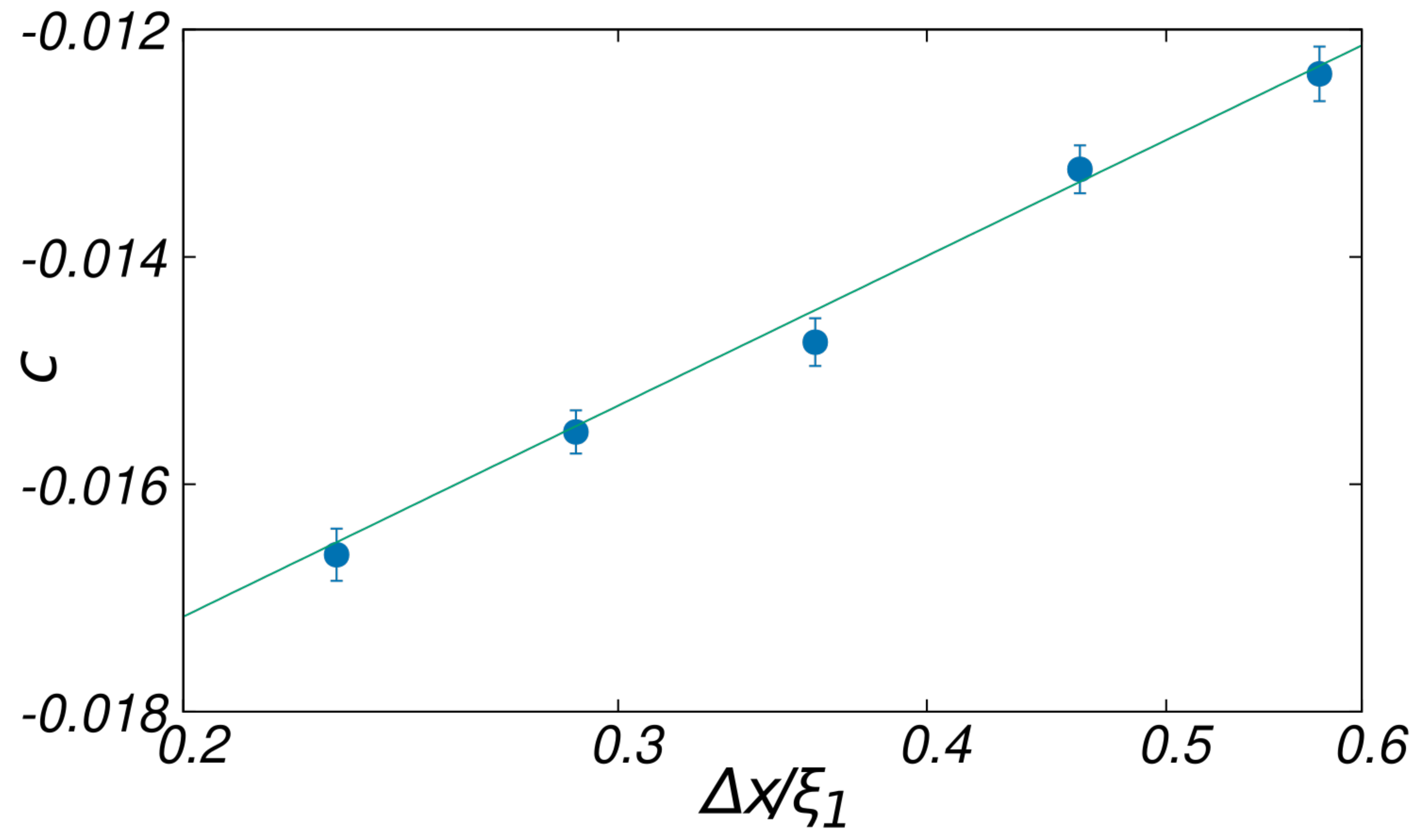
・ Entropy density in $d = 2$:

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

・ 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

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

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

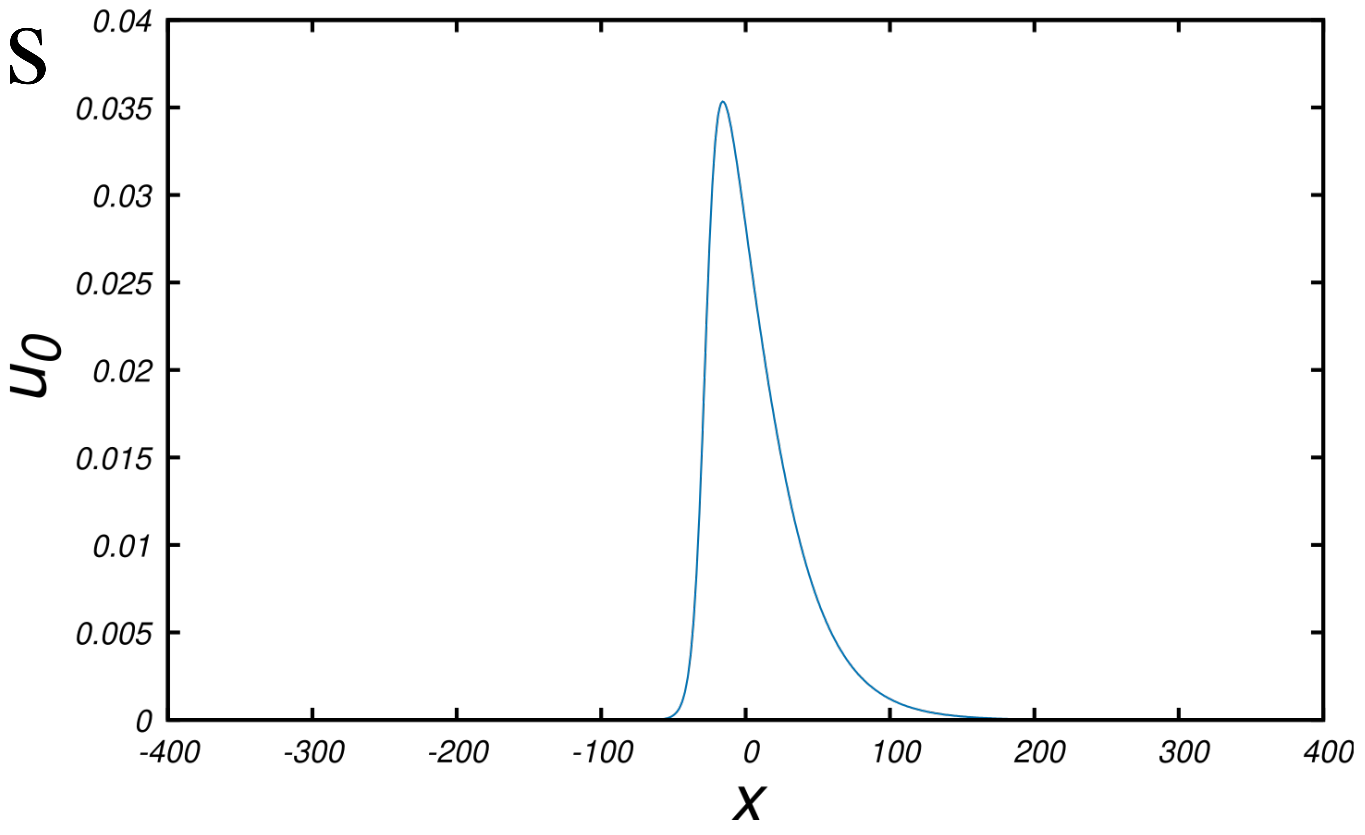
$$(\partial_t - \hat{L}_z - \kappa \partial_y^2)\rho_1(z,t) = \sqrt{2T'}\hat{Q}\eta$$

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

- $(a, b) \equiv \frac{1}{L_y}\int_0^{L_y} dy \int_{-\infty}^{\infty} dx a(x,y) b(x,y)$
- 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

- 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.

Future prospects

- Origin of the cut-off? → Microscopic model

  Lattice gas : H. Spohn, J. Phys. A: Math. Gen. 16, 4275 (1983)

  Potts model : M. Kobayashi, N. Nakagawa, and S.-i. Sasa PRL, 130, 247102 (2023)

- experimental system? → spin-crossover complex

  K. Boukheddaden et.al, Physica B 486, 187-191 (2016)

  S. Miyashita et.al, Prog. Theor. Phys. 114, 719-734 (2005)

  → estimation of cut-off

- Universality class of interface c.f. KPZ equation

- Absence of time-reversal symmetry in Non-eq → New driving force

Conclusion

- 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

SM

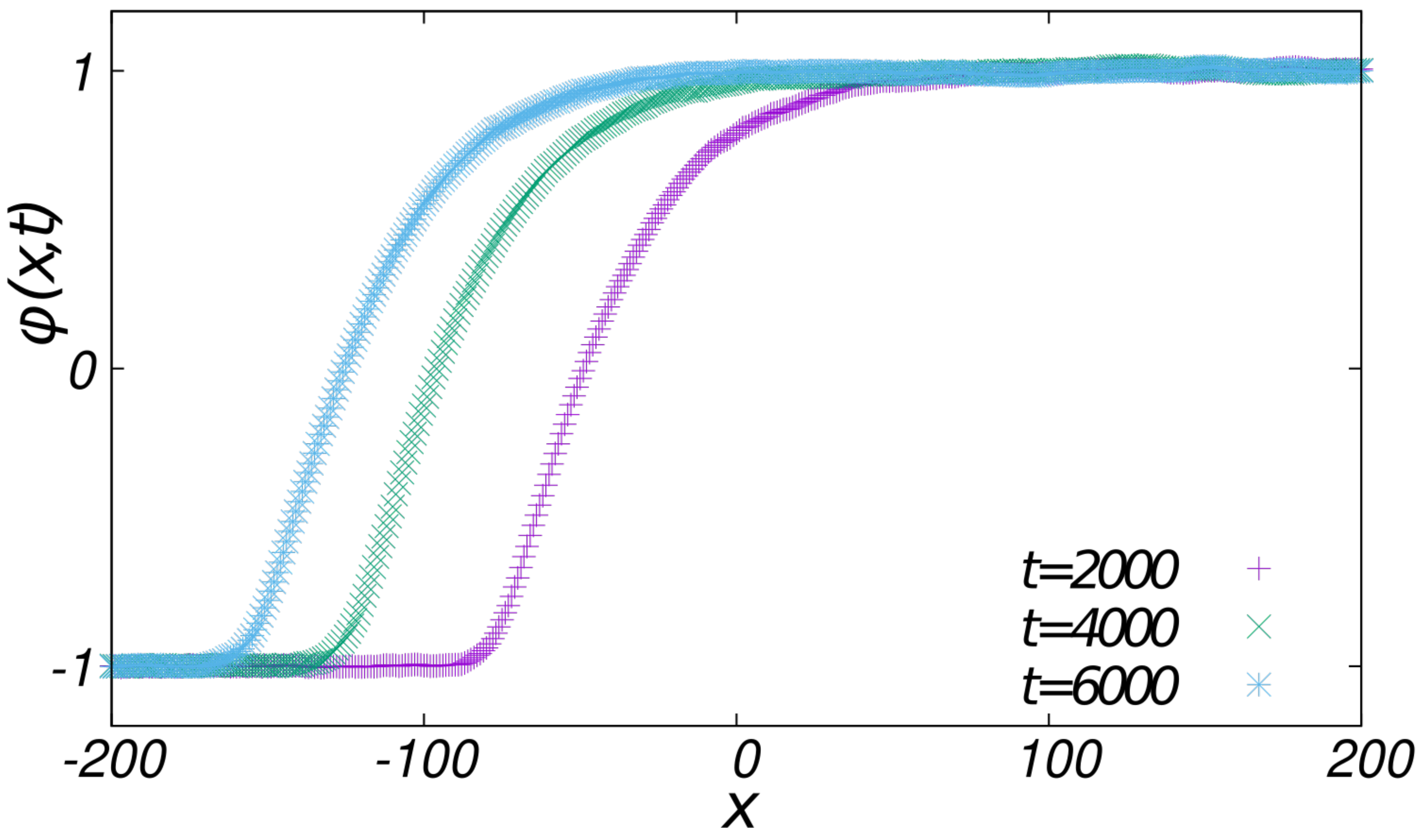
Numerical simulation

- Discretization of space: square lattice
- Time development: Heun method

- Estimation of velocity
  - Order parameter integrated in y :

$$\Phi(x,t) = \frac{1}{L_y}\int_0^{L_y} dy\phi(x,y,t)$$

  - Position of interface $X(t)$:$\Phi(X(t),t) = 0$
  - Time averaged velocity: $V(t) \equiv \frac{X(t) - X(t_0)}{t - t_0}$
  - Estimate c by averaged value $\langle V(t) \rangle$



The case $d = 2$

Numerical scheme

・Discretize $(x, y) \in [-L, L] \times [0, L_y]$ as $(i\Delta x, j\Delta x)$, $-N_x \le i \le N_x, 0 \le j < N_y, N_x\Delta x = L, N_y\Delta x = L_y$

Discrete Laplacian: $\Delta_2 a(i, j) \equiv \frac{1}{\Delta x^2}[a(i+1, j) + a(i, j+1) - 4a(i, j) + a(i-1, j) + a(i, j-1)]$

・Time development: Heun method

$$\phi(i, j, n+1) \equiv \phi(i, j, n) + \frac{1}{2}(h_1(i, j, n) + h_2(i, j, n))$$

$$h_1(i, j, n) \equiv \Gamma[-f'(\phi(i, j, n)) + \kappa\Delta_2\phi(i, j, n)]\Delta t + \sqrt{2\Gamma T}\frac{\sqrt{\Delta t}}{\Delta x}\eta(i, j, n),$$

$$h_2(i, j, n) \equiv \Gamma[-f'(\phi'(i, j, n)) + \kappa\Delta_2\phi'(i, j, n)]\Delta t + \sqrt{2\Gamma T}\frac{\sqrt{\Delta t}}{\Delta x}\eta(i, j, n),$$

$$\phi'(i, j, n) \equiv \phi(i, j, n) + h_1(i, j, n)$$

・Initial condition :

$$\phi(i, j, 0) = \frac{\phi_2 - \phi_1}{2}\tanh\left(\frac{i\Delta x}{40}\right) + \frac{\phi_1 + \phi_2}{2}$$

・Boundary condition in y:

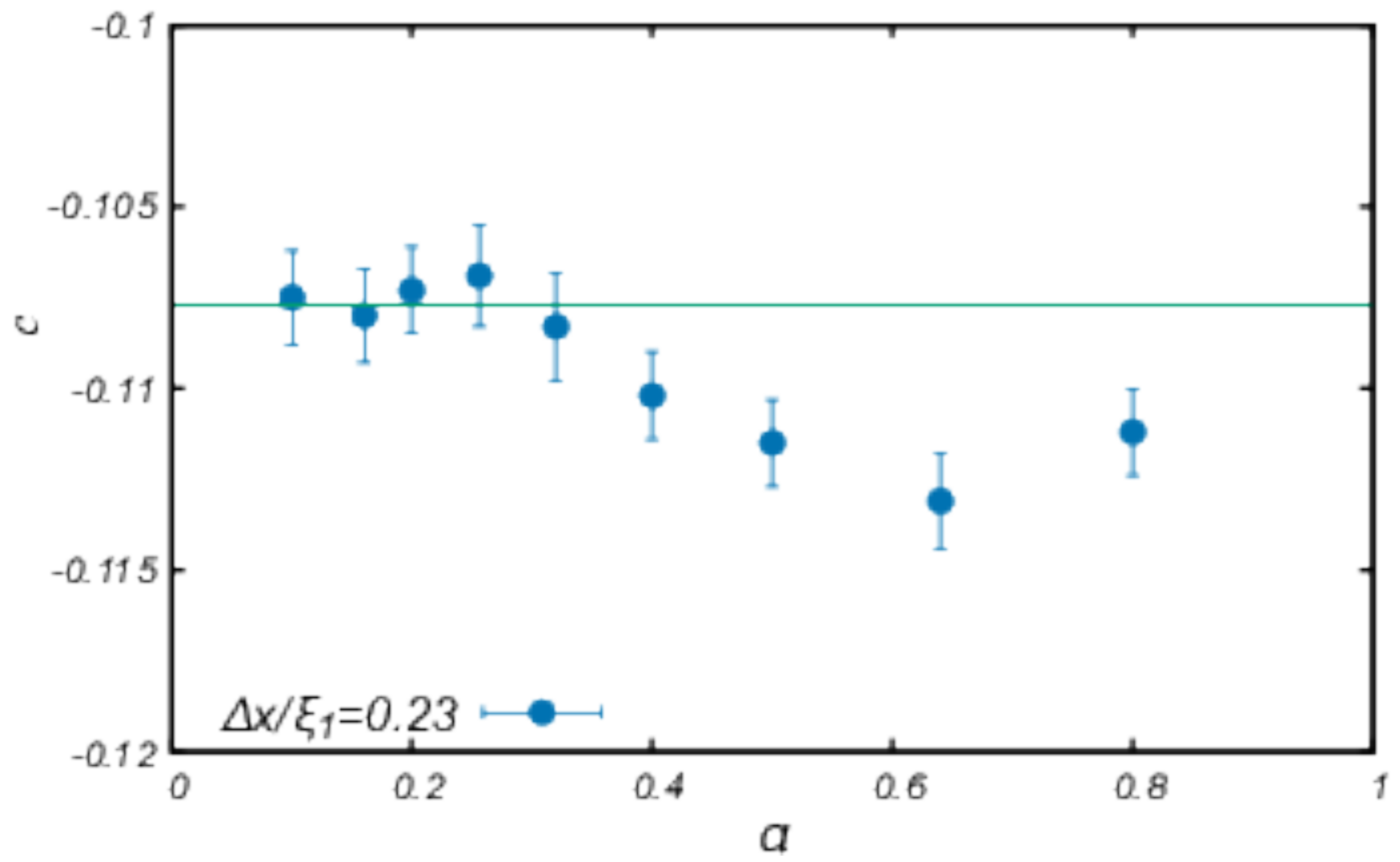
$$\phi(i, j + N_y, n) = \phi(i, j, n)$$

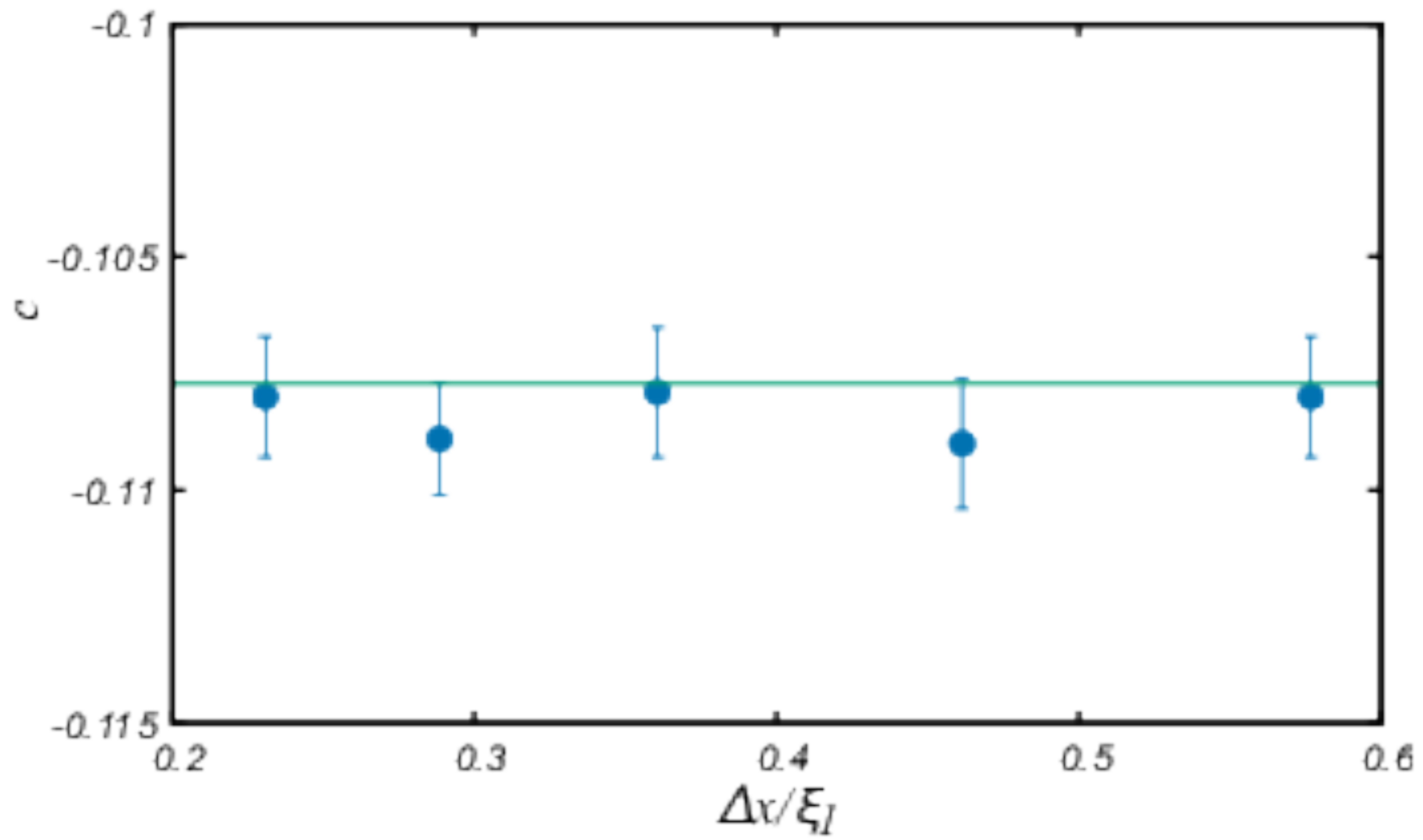
・Boundary condition in x:

$$\phi(-N_x, j, n) = \phi_1, \phi(N_x, j, n) = \phi_2$$

Choice of $\Delta x, \Delta t$

Choose appropriate $\Delta x, \Delta t$ by 1-D simulation





Dimensionless parameter $\alpha = \dfrac{2\Gamma\kappa\Delta t}{\Delta x^2}$, Region$[-800,800]$

changeΔt under $\Gamma = 0.1, \kappa = 1600, T = 0.5, \Delta x = 1$

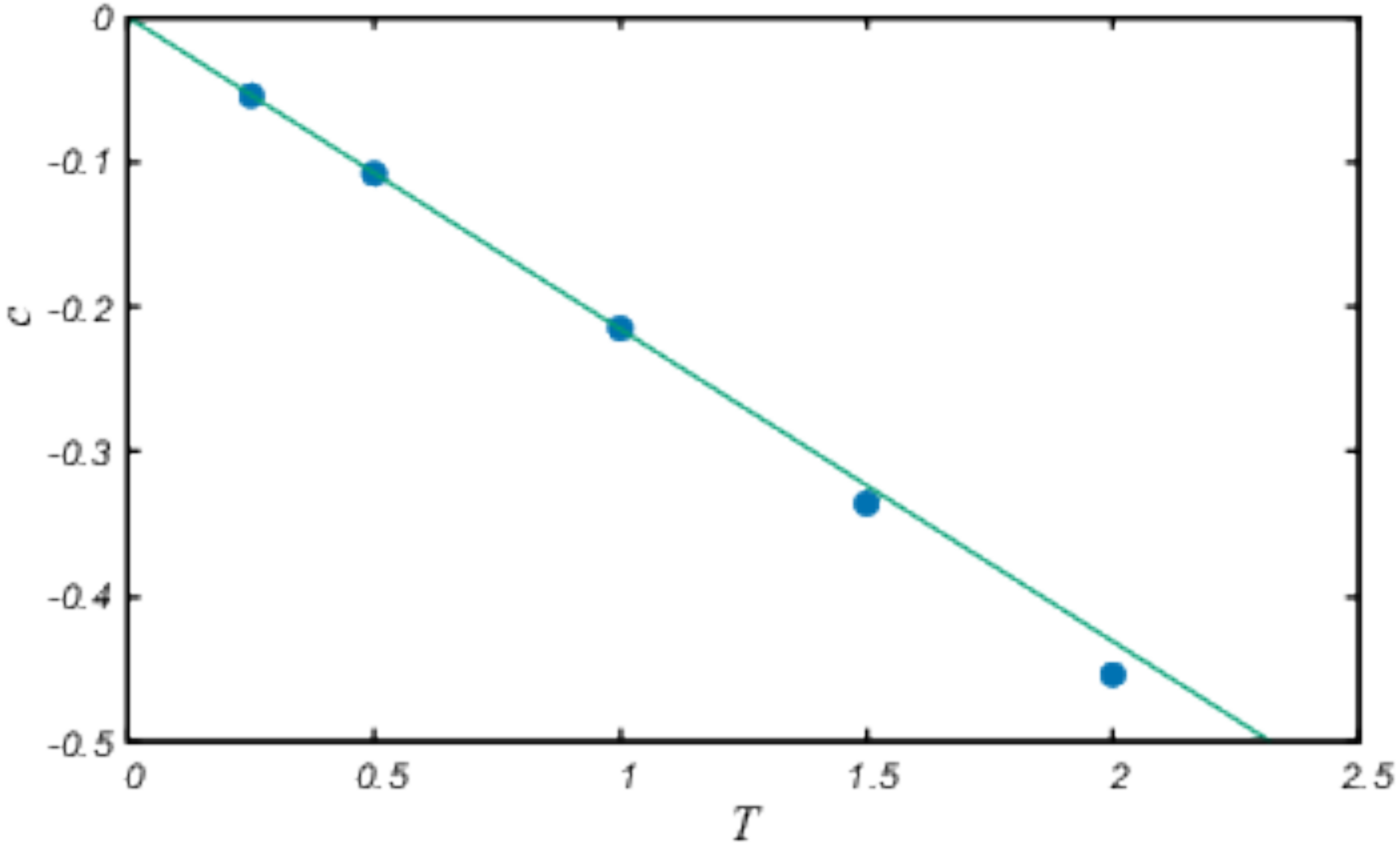
$f(\phi)$: Page 5

Change Δx under $\Delta t = 5.0 \times 10^{-4}$

$\Delta x = 1, \cdots, 2.5,\ \xi_1 = 4.33$

Choice of T

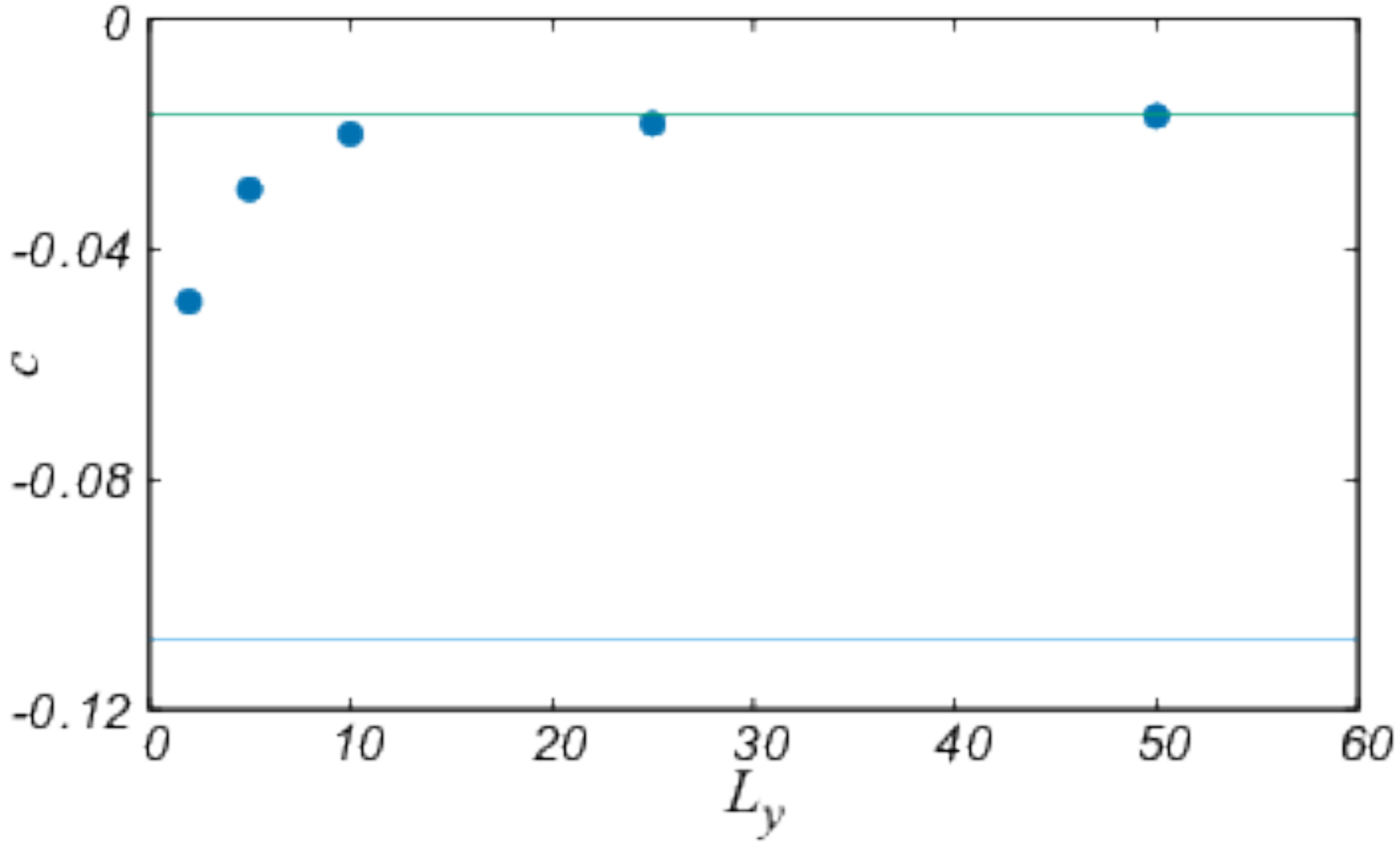
Choose T to which c is proportional.



Change T under $\Delta t = 5.0 \times 10^{-4}, \Delta x = 1.0$, in 1D

Choice of L_y

Confirm the dependence on L_y



Region $[-400,400] \times [0, L_y]$

Change L_y under $\Delta x = 1, \Delta t = 5.0 \times 10^{-4}, T = 0.5$