Analytic and numerical methods for active matter research

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January 6, 2025

Preface

t x ¸ ” 2025D 1Ô 6-9| ÙH Postech | ¤ X APCTPÐ ô ° 22(µ Ä < ¬ ¨ ¸ Y P (22th KIAS-APCTP Winter School on Statistical Physics)X 5Ü Ü ¬ X Ð ð x P ¬… Èä .

¥ Ù < \ À Á t ” < ´ \ l 1 active matter systemsÐ \ µ Ä < ¬ „ | X ð l ” Vicsek, Czirók, Ben-Jacob, Cohen, Shochett 1995D Ð \ \ Physical Review Letters | 8 [VCJ+95]Ð D o È µ Èä . t | 8 @ < ´ X ¥ Ù x ´ Ù 1 (motility)t ä ´ Ä Ñ è Á X ô ¸ 1 D ° X ” u ì x í Y D ôù \ ä” P È D ü à ˆ µ Èä . è X t Ä e ø \ ´ °ü | ô ì ü ” toy model@ J „ Æt \ à Š Ñ Èä . ø X X ˜ D Ð L ˆ X Vicsek ñ X ¨ @ € • ŒÄ \ À 30D t À œ $ ˜ L À Ä µ Ä < ¬ ð l • Ð Œ È \ ´ ð l Ð \ D ˆ ì |< ¤ à ˆ µ Èä . µ Ä < ¬ ð l • ä @ t ` ð l | µ t 9 @ Ý < ä Ø„ | @X Ù ð l | µ t ¥ Ù x ´ Ù 1 t Ì Ü ” È \ ´ Ù í Y < È Á Ü , D É Á t , topological defects, pattern formations ñ D \ ˆ ð l X à ˆ µ Èä .

t X ” ä ‘ \ m 1 D ” active matters ´ p polar order m 1 D ” Ä X D É Á t Ì D ä è à ˆ µ Èä . t ü | …• 0 ð l Ð 0 ø t ” Vicsek ñ X ¨ ü active Brownian particles ¨ D µ t ä ð ƒ …Èä . GPU| \ ©\ molecular dynamics 0 • @ …• 0 ¨ Ä X Á t | ä è ” %\ X ð l)• … Èä . \ ¸ Boltzmann) Ý ü Smoluchowski) Ý @ …• 0 ¨ Ä | ì ì À t ` x ð l )• D ©` ˆ ” continuum) Ý < \ 0 ` ˆ Œ t Èä . X | µ t • 8 ˆ Œ ` P)• ` t active matters Ð Ì D È | ä x ð l „ |Ð Ä \ ©` ˆ 8 0 i Èä .

äµ D Ð X ” „ ä D t CUDA\ ‘ 1 molecular dynamic simulation \ ø ¨ ü python3\ ‘ 1 animation \ ø ¨ D õ X µ Èä . CUDA \ ø ¨ D ¬ © X 0 t ” C 9 @ C++ ¸´Ð \ À Ý t D ” X p Nvidia X gpu D ” i Èä [8 à : https://sites.google.com/view/jdnoh-tcp/cuda-gpu]. Animation \ ø ¨ D ¬ © X 0 t ” python3@ C/C++ compiler D ” i Èä . $ ¸ Ì l | µ t t ä ° • ÐÐ ü ` ˆ ” X ½D ø ¬ È (t “ 8 • Èä .

t X x ¸ ” ì ì review papers| 8 p X ì ‘ 1 ˆ LD ™Èä [MJR+13, PBGC14, Cha20].

Contents

1

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1.1 Active matter란?

à x ä´ Ä| l 1 X” …•X Ùí Y D Ý t ô • . à ½ Ä Ð …•X ´ Ù@ ° ` x ´ Ù) Ý D 0 x ä . Ä ô x 9 @ D ô x x € X ½ü Á 8 ‘ © X à ˆ ä t …•X ´ Ù@ U ` x •1 D Ä Langevin) Ý < \ 0 ä . | ä ´ (Ä Tt à damping coefficient $1/\mu$x ´ Ð Brown …• ” x % Ð à Ä ä È D l 1 X ” …• ä ü X 4 ‘ x © Ì X ¥ D ”ä . Overdamped limitÐ Brown …• iX X $\boldsymbol{r}_i$” ä LX stochastic Langevin) Ý D 0 x ä :

$$\dot{\boldsymbol{r}}_i = \mu \boldsymbol{F}_i + \sqrt{2D}\boldsymbol{\eta}_i(t) \quad \left[\text{diffusion constant } D = \mu k_B T, \langle \eta_i(t) \rangle = 0, \langle \eta_i(t)\eta_j(t') \rangle = \delta_{ij}\delta(t-t')\right]. \tag{1.1}$$

Ì } Brown …• 3X x € X ½< \ € 0 Ð À| a X ì t | í Y Ð À\ X ` ˆ ä t , …• ” stochastic noise $\boldsymbol{\eta}$Ð X \< Ù x ´ Ù Ð T t • t à ¥ Ù x ´ Ù D ` ˆ Œ ä . ¥ Ù´ Ù X • %D v_0,) ¥ D è ¡ 0 $\boldsymbol{n}$\ ˜ À´ t …•X ´ Ù) Ý @

$$\dot{\boldsymbol{r}}_i = v_0 \boldsymbol{n}(t) + \mu \boldsymbol{F}_i + \sqrt{2D}\boldsymbol{\eta}_i(t) \tag{1.2}$$

X 4 D Œ p , v_0@ n \ • ´ X Ùí Y D Œ ä . • x ´ Ù 1 (motility)D ” …• \ l 1 < È D ¥ Ù < È (active matter)t | € x ä .

¥ Ù < È t D Ì ½° Ð Ä …• ä @´ Ù 1 D È ˆ ä . ^ Œ \ Brown …• ø \ x t p , D É µ Ä í Y Ð Tˆ ä è ” driven lattice gas systems í Ü À Á t ” …• \ t è ´ 8 ˆ ä . Motility@ mobility| D ½ˆ | ˆ ” l „ D Ü X 0 ” ´ 5 À Ì , ´ < \ ¥ Ù < È @ persistence •1 t ˆ ” …• \ l 1 Ä | À m\ ä .

¥ Ù < È X ” • ð Ä , ¹ ˆ Ý < Y Ä Ð } Œ > D ˆ ä . 8 ì ´ X active cytoskeleton€ 0 D äÈ” È Ð t t ” Ý < Y x ¥ Ù < È Ä ” Ý T Y Ð À | motilityX Ð Ì\ ¼”ä . Á t \ T Y p 1 D ” ‘ t < \ t è ´ Ä Janus particle, • 0 ¥< \ l Ù ” Quincke roller, 0 Ð À \ l Ù ” \ ñ @ x õ < \ i 1 ¥ Ù < È X \ ä Ø ð l Ð \ © à ˆ ä .

1.2 Ñ 단거동Ð 대\ µ 계< 리 ð 구 P 름

p Ü Ä X Ñ è p Ù Ð \ µ Ä < ¬ ð l X P „ D è T t 0 t ô • . µ x µ Ä < ¬ Y X 4 ” © • (lattice) ä . © • Ð à ´ ˆ p ˜ © • ¬ t | t Ù X ” …• 9 @ ¤ @ä X Á t @ Ù í Y • ™ Á Ð \ ð l \ X Œ Ä ‰ È à , ø °ü \ õ X (Ð , m 1 , ô t • Y ñ t p Ü Ä Ñ è p Ù X ô ¸ 1 D ° X ” ” \ ” Œ„D L Œ È ä .

õ ¡ ð ° Ý ¹ ˆ ™Ä Æ” ð ° Ý X ¬ @ µ Ä < ¬ Y X 4 | T ± U ¥ Ü 0 ä . õ ¡ ð ° Ý X x Ü Ð à 9 @ Á l | µ t ´ Ù X ” …• @ ¤ @ä D ¬ © t ä ‘ \ ð l Ä ‰ È à , t ì \ Ü Ä ” µ Ä < ¬ Y X ” ü | õ Y /x 8 /¬ Œ„ | X õ ¡ Ä Ð L À ä .

1 `

¥ Ù < È Ä ” …• 9 @ ¤ @X ´ € Á Ü @ T ˆ ´ X L À Ù í Y x À ä” Ð µ Ä < ¬ Y ð l X È \ ´ (ì ä „< \ • ¬ ¡ à ˆ ä . ¥ Ù < È Ä Ð ” …•X õ x • Ä @ ¤ @ ñ X ´ € • Ä X Œ ° i ´ ˆ ä . t Ð à $ À JX X È \ ´ …X X ° i @ µ Ä < ¬ Y ð l • Ð Œ Î @ ð l ü | X 8ü à ˆ ä .

2

Vicsek model

2.1 Vicsek model

Vicsek ñ @ È 4 ¬ X ¼À L Á D $ …X 0 t [1] "self-driven particles"\ t è ´ Ä ¨ Ä | Ä …X à Monte Carlo simulation ð l | ‰X ì » @ È \ ´ …X X Á t | ô à X ä [VCJ+95]. t ù | 8 X • " 5…t À Ì , ¨ à 8 Ì Ð ø ï t | 8 Ð Ü \ ¨ D Vicsek ¨ t | € t ä . Vicsek ¨ X ¹ Õ D ¬ t ô • .

- L^2 l 0 X 2(Ð É t Ð $N = \rho N^2$ X …• \ l 1
- …• iX Á Ü " X $\boldsymbol{r}_i(t)$@ • Ä $\boldsymbol{v}_i(t) = v_0(\cos\theta_i(t), \sin\theta_i(t))$\ t À à , • %@ $|\boldsymbol{v}_i| = v_0$\ | X ä .

[1] ¼À ´ äÈ" Ù < Ð \ artificial life ¨ @ 1986D Ð ° ü Y •x Craig Reynolds Ä …\ ˆ ä . Boid = B(irds) + (andr)oid\ ……\ ¨ (• Ì " https://www.red3d.com/cwr/boidsÐ U x ` ˆ ä .

- $\Delta t = 1$X Ü © ÙH ¨ à …•X X@• Ä ÙÜÐÅ p t ¸ ä .

$$\boldsymbol{r}_i(t+1) = \boldsymbol{r}_i(t) + \boldsymbol{v}_i(t), \quad \theta_i(t+1) = \mathrm{Arg}\left[\sum_{j\in\mathcal{N}_i} e^{i\theta_j(t)}\right] + \xi_i(t) \tag{2.1}$$

$\mathcal{N}_i$: …• i@X p ¬ $r_0 = 1$ô ä '@ …• ä X Ñi

$\xi_i(t)$: uncorrelated random noise uniformly distributed in the interval $[-\eta : \eta/2]$

- …• " • àX • Ä) ¥D ü …•X Éà ´ Ù) ¥ü , Xà• \ ä .

- • Ä , Á8 ' ©@ \\ p ¬ $r_0 = 1$´ Ð Ì ' ©X" **short range interaction**t ä .

- • Ä , Á8 ' ©@• Ä) ¥ Ä θ| „XX Ä ϕÌ | TX" $(\theta \to \theta + \phi)$ ð• x Œ ÀXÐ t m t ä .

- …•X motility| xXt …•X • Ä) ¥ Ä" • 1 XY ¨ ü @ m1D "ä .t ì \ t \ Vicsek ¨ X…• | flying XY spin, Vicsek ¨ D active XY ¨ t | à €t 0Ä \ ä .

• 1 •1 D " alignment Á8 ' ©@ ¨ à …• @) ¥<\ ÀÁt " ¼ÀL (flocking) Ñèp ÙD |< ¬ ˆ ä . ´ …•X Éà • Ä" ¼ÀL ÁX order parameter í ` D \ ä .

$$v_a = \frac{1}{N v_0}\left\langle\left|\sum_{i=1}^{N} \boldsymbol{v}_i\right|\right\rangle_s \tag{2.2}$$

1995DX | 8Ð • ä @ …• Ä ρ@ aligning interactionD) tX " ¡LX l 0 η| Ô p XÄ° D ‰Xì ä L ü @° ` D »È ä .

- Ä ®à ¡LX l 0 p íÐ Ä” $v_a = 0$x disordered (gas) phaseÐ ˆ ä .
- Ä ’ à ¡LX l 0 ‘@ íÐ Ä” m1 t• <\ h Ä $v_a \neq 0$x ordered (flocking) phase Ð ˆ ä .
- gas phase@ flocking phase ¬ t Ð” order-disorder ð • Á t | ´ œä .

$$v_a \sim |\eta_c - \eta|^{0.45\pm0.07}, \quad v_a \sim |\rho - \rho_c|^{0.35\pm0.06} \tag{2.3}$$

t °ü ” ä ä € | € D X p active matters µ Ä < ¬ „ | X ” ð l ü \ € Á X ” p ° x Ä 0 È ä .

2.2 Mermin-Wagner theorem

Mermin-Wagner (9 @ Hohenberg-Mermin-Wagner) ¬ ” ü p ¬ Á 8 ‘ ©X à ð • m1 t ˆ ” ô É Ä Ð t ä L ü t ü ¥ \ ä : **“Continuous symmetries cannot be spontaneously broken at finite temperature in systems with sufficiently short-range interactions in dimension** $d \leqslant 2$**”** [Hoh67, MW66].
d(Ð ©• Ð X XY ¨ D µ t ¬ X X ø | t tt ô • . XY ¨ X t È H @

$$H = -J \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j) \quad \text{[ferromagnetic coupling constant } J > 0] \tag{2.4}$$

t ä . t t È H @ nearest neighbor interactionÌ D ì hX à ˆ à ¤ @ Ä | „XX Ä ϕ\ Œ t Ù X ” ð • À X Ð t ˆ À x $U(1)$ m1 D à ˆ ä .

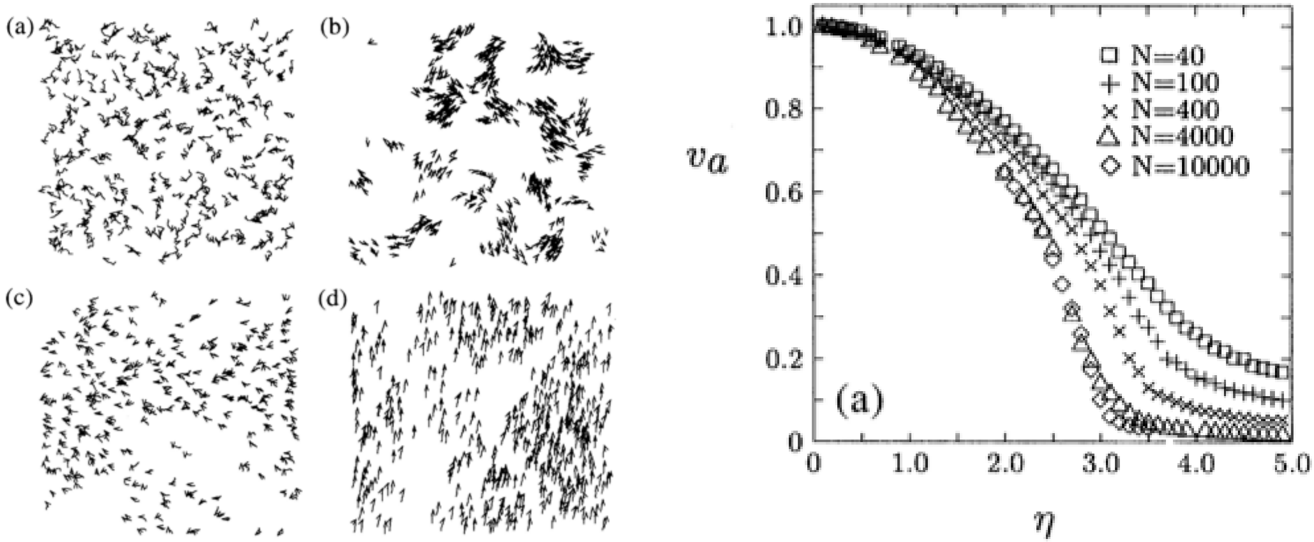

Figure 2.1: Vicsek ¨ X snapshotü order parameter scaling. (8 à 8 Ì [VCJ+95]Ð Ì h .)

XY ¨ X ground state" ¨ à ¤ @t | ,\ , $(\theta_i^g = \theta_0)$ • 1 Á Ü , ‰ $U(1)$ m1 t • < \ h Ä Á Ü t ä . • 1 Á Ü ô " Ù Ð ´ D¨ " À | ´ ´ ô 0 t p Ü x p ¬ LÐ x Ð ¤ @ Ä 2πÌ | ´ ˜ " spin wave excitation $\theta_i = \theta_i^g + 2\pi x_i / L$ D à $ t ô • . Lt p ½° spin wave excitationX Ð À "

$$\Delta E \simeq \frac{J}{2} \sum_{\langle i,j \rangle} (\theta_j - \theta_i)^2 \simeq J a^2 L^{d-2} \tag{2.5}$$

t ä . $d \leqslant 2$| L t @ 0< \ 4 X p ˜ \\ < \ 4 \ ä . 0 | (Ä 0t D È t ô " Ù < \ Ý 1 U ° spin wave excitationst • 1 È | 4 \ ä . ½Ä Ð ˆ " $d = 2$ (Ð @ ¹ Ä \ ½° Ð t ù ´ , long range ferromagnetic order" 4 À Ì ¤ @-¤ @ Á Ä h power law| 0 t " quasi long range ordered Á Ü ¥ X ä [JKKN77].

^ ´ ´ ø @ t Vicsek ¨ @ XY ¨ ü @ m1 D " active XY ¨ Ð t ù \ ä . Vicsek ¨ Ð ¬ flocking phase" Mermin-Wagner ¬ Ð X t ô É Ä Ð " t ¬ ` Æ@ È \ ´ < È Á Ü x ƒ t ä . Mermin-Wagner ¬ X \ D h à ð • x Œ m1 t • < \ • 4 " ü Ð @ 4 Ç | L ?

Tasaki" Mermin-Wagner ¬| flocking ¨ < \ U ¥ X $ " Ü Ä | ˆ ä [Tas20]. X $\boldsymbol{r}_i$, • Ä $\boldsymbol{v}_i$X •1 D " N X …• t t L^2x 2(Ð õ Ð ˆ ä . Ä X t È H @

$$H = \left[\sum_{j=1}^{N} \epsilon(|\boldsymbol{v}_j|) + \sum_{j \neq k} u(\boldsymbol{r}_j, \boldsymbol{r}_k) \right] - \sum_{j \neq k} J(\boldsymbol{r}_j, \boldsymbol{r}_k) \frac{\boldsymbol{v}_j}{|\boldsymbol{v}_j|} \cdot \frac{\boldsymbol{v}_k}{|\boldsymbol{v}_k|} \tag{2.6}$$

t à (u: hard core repulsion, $J > 0$: short-range alignment interaction kernel), • Ä) ¥ D „XX Ä \ Œ X " ð • À X Ð t ˆ À x m1 D "ä . Tasaki" McBryan-Spencer bound| " Y L Ì É D ¬ © X ì

(Ä $1/\beta$x ô É ÁÜÐ p¬ lÌ | ¨ ´ Ä P …•X • Ä-• Ä Á Ä h Ì q X” € ñ Ý

$$C_l(\beta) := \frac{1}{Z(\beta)} \int d\boldsymbol{R} d\boldsymbol{V} \left(\frac{\boldsymbol{v}_j}{|\boldsymbol{v}_j|} \cdot \frac{\boldsymbol{v}_k}{|\boldsymbol{v}_k|} \right) e^{-\beta H} \leqslant \left(\frac{l}{a_0} \right)^{-\eta} \tag{2.7}$$

D »È ä (η” ‘ X Á). t °ü ” …•X ´ Ù1 t ð• m1 D Dð < \ • 4 Ü¤ À” J ä” ƒ D X ø \ ä . TasakiX °ü ” flocking order| ” Vicsek ¨ X °ü @‘ ½` ˆD L ?

2.3 Toner-Tu t 론

Vicsek ¨ | 8 t \ t Ð Toner@ Tu” Á` x¥ ) ÝD ÜXà renormalization group (RG) „ D ‰X ì 2( ÐÐ long range flocking order t ¬` ˆLD ü¥ X ä [TT95, TT98]. …•X Ä $\rho(\boldsymbol{r},t)$@ • Ä $\boldsymbol{v}(\boldsymbol{r},t)$ fieldÐ \ Toner-Tu) Ý@ ä L ü ä .

$$\partial_t \rho + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{v}) = 0 \tag{2.8}$$

$$\begin{aligned} &\partial_t \boldsymbol{v} + \lambda_1 (\boldsymbol{v} \cdot \boldsymbol{\nabla}) \boldsymbol{v} + \lambda_2 (\boldsymbol{\nabla} \cdot \boldsymbol{v}) \boldsymbol{v} + \lambda_3 \boldsymbol{\nabla} |\boldsymbol{v}|^2 = \\ &\quad \left\{ \alpha - \beta |\boldsymbol{v}|^2 \right\} \boldsymbol{v} - \boldsymbol{\nabla} P + D_0 \boldsymbol{\nabla}^2 \boldsymbol{v} + D_1 \boldsymbol{\nabla} (\boldsymbol{\nabla} \cdot \boldsymbol{v}) + D_2 (\boldsymbol{v} \cdot \boldsymbol{\nabla})^2 \boldsymbol{v} + \boldsymbol{f}. \end{aligned} \tag{2.9}$$

$\alpha > 0$| L t) Ý@ homogeneous ordered stateÐ t ù X” t $\rho(\boldsymbol{r}) = \rho_0$, $\boldsymbol{v} = v_0 \boldsymbol{e}_x$| ”ä . Toner-Tu” | (X ü¬ | µ t homogeneous ordered state\ € 0 X ” Ù $\rho = \rho_0 + \delta\rho$, $\boldsymbol{v} = (v_0 + \delta v_\parallel)\boldsymbol{e}_x + \delta \boldsymbol{v}_\perp$X Á Ä h anisotropic power law scalingD 0 „ D ô ä .

$$C(\boldsymbol{R}) := \langle \boldsymbol{v}_\perp(\boldsymbol{r}+\boldsymbol{R},t) \cdot \boldsymbol{v}_\perp(\boldsymbol{r},t) \rangle = R_\perp^{2\chi} F_V \left(\frac{R_\parallel}{R_\perp^\zeta} \right) \tag{2.10}$$

\ RG Ä ° D µ t 2(ÐÐ roughness exponent χ@ anisotropy exponent ζX U\ D l ˆ ä .

$$\chi = -\frac{1}{5}, \quad \zeta = \frac{3}{5} \tag{2.11}$$

Roughness exponent LX D 0 Ð • Ä X " Ù @ p ¬ @´ È] ´ à ä . ‰, " Ù t flocking ordered state| 4 ` ÆLD X ø \ ä . Toner-TuX °ü " Mermin-Wagner ¬| 0 t " ô É Ä Ð @"ì ¬ active matterÐ ð • m1 t • < \ • 4 ˆLD t < \ ô x \ X Å < \ ü à ˆ ä .

ø ì ˜ , Toner-TuX t ` @ À ˜ X Œ Á ` t à l ´ x ¨ Ä T X Ä ˆ„ …X ä" è D à ˆ ä . T p ä ˜ Toner" 2012D Ð œ \ | 8 Ð Toner-Tu ¨ Ð à $ X À J @ È \ ´ D mD " \ Ä …X t Toner-Tu RG Ä ° X Ä 1 t ¬| ÐD ô ä [Ton12]. 0 | Toner-TuX t ` @ Mermin-Wagner ¬ @ @ Ä \ t ` < \ D ä t 0 ô ä" ü ¬ x t ` < \ D ä t " ƒ t À ù X ä .

2(Ð Vicsek ¨ X ordered phase íÐ X < \ Ä ° \ Á Ä h " Ý (2.10)ü @ anisotropic power law scalingD 0 x ä [MGC19]. è , „ Ä À X @ $\chi = -0.31(2), \zeta = 0.95(2)$t p Toner-TuX ü } X (t | ô x ä .

2.4 ð • Á tx 가 ˆ ð • Á tx 가?

• ð • m1 • 4 @ T ˆ ´ flocking Á tX •1 \ | € D ˆ ì |< 0 ä . Vicsek ø ù @ 1995D X | 8 t ˜ \ flocking Á t ð • Á t | à ü ¥ X ä (Ý (2.3) 8 p). ø ì ˜ , p l 0 Ð 4 Ü Ù H ‰ X Ä ° @ flocking Á t ˆ ð • Á t„D ô ì ü È ä . e ø mŒÄ (ρ_0, η) É t Ð X Á É ø ¼@ a ´ -0 ´ Á t | ª " ´ X Á É ø ¼ü ¬ X ä [Cha20].

- homogeneous disordered (gas) phase ($v_a = 0$): Ä @ • Ä X Á Ä À h < \ Œ\ ä .
- polar ordered/homogeneous ordered/flocking (liquid) phase ($v_a > 0$): …• ä t Ñ è < \ \ ) ¥ < \ ´ Ù \ ä . …• ä @ Ä Ð à | X Œ „ ì X À Ì …• Ä ” X Œ ” Ù \ ä (giant number fluctuation). ‰, t t ξ^2x íÐ ì h …• | n_ξ| ` L , …• X ¸ (power law scaling $\langle(\delta n_\xi)^2\rangle \sim \langle n_\xi\rangle^\alpha$D 0 t p 2(Ð Ð „ Ä À ” $\alpha = 8/5$ (Toner-Tu), 1.67 (simulation)t ä [MGC19].
- band (coexistence) phase: 0 ´ Á Ü @ a ´ Á Ü \ Á „ ¬ (microphase separation) | ´ œä . Á „ ¬ a ´ ” ¡ < \ ¼Ð Ä ` (bands) ¨ ‘ < \ 0 ´ Á Ü | 0 ½< \ ´ Ù \ ä . a ´ ` X í ü © @ \X ä .

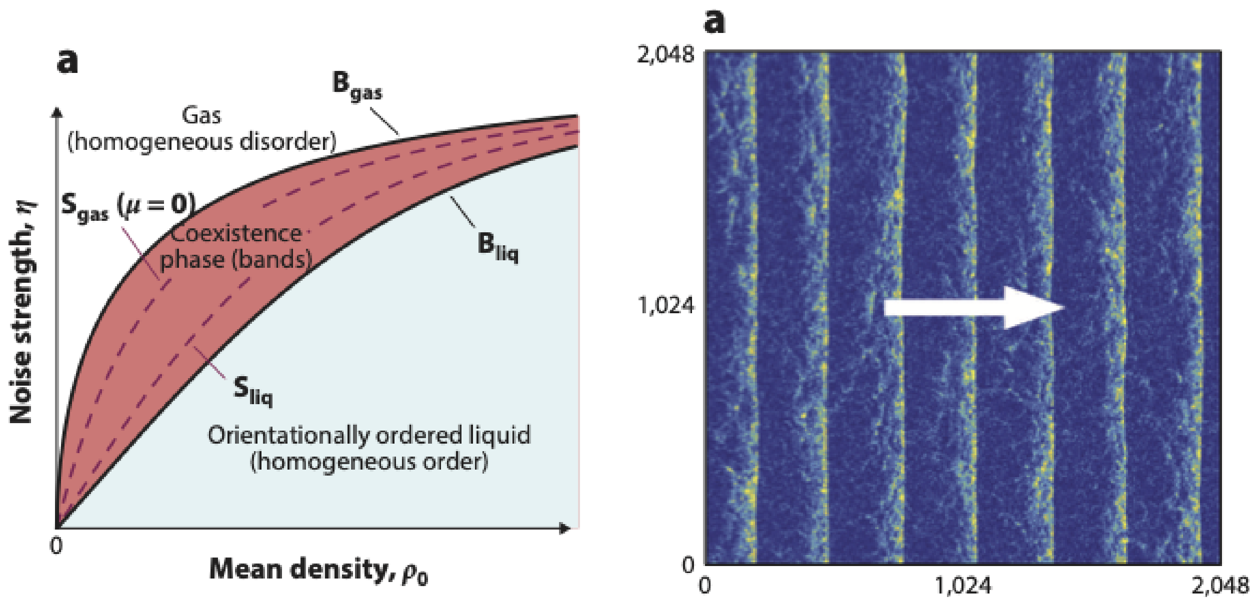

Figure 2.2: Vicsek ¨ X Á É ø ¼ü õ t Á Đ X ` l p ([Cha20]Đ Ì)

3

X ð 구)•

3.1 Self-propelled particle 모

…• 0 X active matter ¨ ´ p ¥ \ x ƒ t self-propelled particles (SPP) ¨ t ä . …•X Á Ü ” X ¡ 0 @ • Ä ¡ 0 X $(\boldsymbol{r}, \boldsymbol{v})$< \ ü ´ À à , t ä @ ¨ Ä X ¹ 1 D X ì p ¬ @ • Ä Ð 9 @ h Ø X t X ” Á 8 ‘ ©D ü à < p Ü Ð 0 | À T \ ä . …•X • %@ Tˆ Á v_0\ è X à , • Ä X) ¥ @ polar angle $-\pi < \theta \leqslant \pi$\ \ Ü \ ä . ‰, $\boldsymbol{v} = v_0 \boldsymbol{n}(\theta)$t à $\boldsymbol{n}(\theta) = (\cos\theta, \sin\theta)$” • Ä) ¥ X è ¡ 0 t ä .

3.1.1 Vicsek-type 모

- discrete time $t = n \times \Delta t$, continuum space $\boldsymbol{r} \in \mathbb{R}^2$

- è p ¬ • Ä , Á 8 ' ©D ì h\ ´ Ù) Ý

$$\boldsymbol{r}_i(t+1) = \boldsymbol{r}_i(t) + v_0 \boldsymbol{n}(\theta_i(t)) \tag{3.1}$$

$$\theta_i(t+1) = \mathrm{Arg}\left[\sum_{j \in \mathcal{N}_i(r_0)} e^{i\theta_j(t)}\right] + \xi_i(t) \tag{3.2}$$

$\mathcal{N}_i(r_0)$" …• i\ € 0 X p ¬ r_0 t X x …• ä Ñi D ˜ À´ à , $\xi_i(t)$" l $[-\frac{\eta}{2} : \frac{\eta}{2}]$ ¬ t Ð à | X Œ „ ì X à Á Ä Æ" ¡LD ˜ À¸ ä .

3.1.2 Active Brownian Particle (ABP) 모

- continuous time, continuum space $\boldsymbol{r} \in \mathbb{R}^2$
- è p ¬ Á 8 ' © ì P \ *W*ü • Ä , Á 8 ' ©D ì h\ ´ Ù) Ý

$$\begin{aligned} \frac{d\boldsymbol{r}_i}{dt} &= v_0 \boldsymbol{n}(\theta_i) - \nabla_{\boldsymbol{r}_i} W + \sqrt{2D_t}\zeta_i(t) \\ \frac{d\theta_i}{dt} &= -\frac{J}{|\mathcal{N}_i(r_0)|} \sum_{j \in \mathcal{N}_i(r_0)} \sin(\theta_i - \theta_j) + \sqrt{2D_r}\xi_i(t) \end{aligned} \tag{3.3}$$

- …• ¬ t Ð è p ¬ ™%t ' ©X à • Ä , Á 8 ' ©t ÆD L $(J = 0)$, ABP ¨ @ motility-induced phase separation (MIPS) Á D |< ¨ ä [FM12].

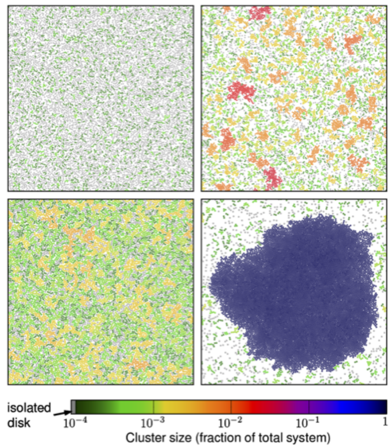

Figure 3.1: ABPÐ | ´ ˜ ” MIPS ([FM12]Ð Ì).

3.2 Molecular dynamics L 고리듬

…• 0 ¨ Ð \ „ • Ùí Y L à ¬ ì D LD ô • . SPPX ´ Ù) ÝD X „ ` L ¥ ´ $´ |@ è p ¬ Á 8 ‘ ©X I 0 | Ä ° X ” ƒ t ä . Ì } …•X Á 8 ‘ © Ý $\mathcal{N}_i(r_0)$D I X 0 t ¨ à …•X X | € \ ä t è Ü © $\Delta t$ ÙHÐ ‰t | X ” Ä ° ‘ @ ´ …• / X ñ $N^2$Ð D@` ƒ t ä .t Ä ° D ¨ (< \ ‰X ” ƒ t „ • Ùí Y Ä ° X u ì ü t ä .

3.2.1 Cell linked-list

Cell linked list 9 @ cell list| ¬ ©X t ü p ¬ Á 8 ‘ © Ä ° Ð D” \ Ä ° ‘ D $O(N)$< \ • 0 < \ | ˆ ä [1]. ø ¼ 3.2X 2(Ð | ô p cell linked-list| Ì Ü” ü D ´ ´ ô • .

1. 4×4X 2(Ð õ Ð 8 X …• „ ì X à ˆ ä .
2. ´ õ D $r_0 \times r_0$| 0 X cellä \ „ `\ ä . $r_0 = 1$x ½° 16 X @t Ý 4 ä .
3. …•X @ ü Œ| Ä ° \ ä (0ˆ …• →10ˆ @, 1ˆ …• →4ˆ @, ...).
4. …• ä D @ ü Œ 0 < \ sortingX à , …•X x q ¤ | @ ü Œ \ ¬ $ \ ä .
5. @Ð ì h …•X 8 ¬ ˆ 8 @ , ¬ ˆ 8 | ¥ \ ä (1ˆ @Ð” 0 ∼ 0ˆ …• , ..., 10ˆ @Ð” 4 ∼ 5ˆ …• , ...). D´ ˆ ” @X 8 ¬ ˆ 8 @ , ¬ ˆ 8 ” NULL\ $ \ ä .

t ü D ÈX t (i) …• ” ¨ à •1 D ô t \ D\ x q ¤ Ì à (ii) @@ • à Ð ì h …• ä X ©] (8 ¬ ˆ 8 @ , ¬ ˆ 8 ¬ t)D Œ ä .

3.2.2 Á 8 ‘ © Ý > 기

Cell linked list| ¬ ©t …• iX Á 8 ‘ © Ý D > ”)• D LD ô • . í Ü ø ¼ 3.2X 2(Ð | µ t $ …X ä .

[1]D • ” cell listÐ 0 \ „ • Ùí Y 0 • D 2012D 1Ô 30| Ð 2Ô 3| ÙH POSTECHÐ ô ° 9(µ Ä < ¬ ¨ ¸ Y P Ð 0 à ä . %X à ©\ X Ä ° • D L $ ü à KISTIX à ¬ Ø Ä ì < \ ¬ X x ¬ | , ° ä .

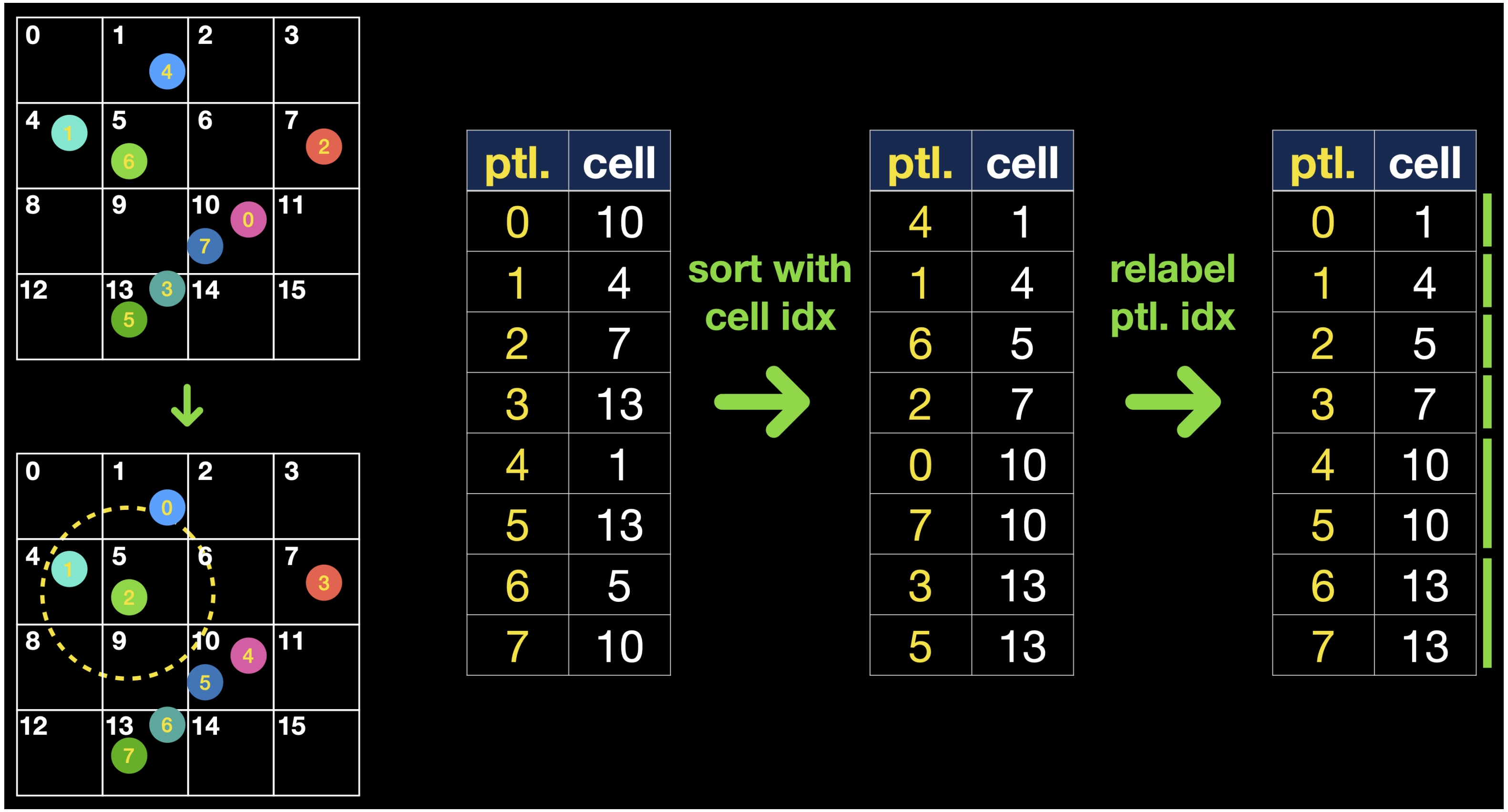

Figure 3.2: Cell linked-list Ì ä 0 .

- …• *i* • \ cellü ü X X ì ø à ˆ ” cell 9 | à $ \ ä . ($i = 2$t t $\{0,1,2,4,5,6,8,9,10\}$)
- @Ð ¥ …•X 8 ¬ , , ¬ ˆ 8 ô | ¬ © X ì 9 @Ð ì h ¨ à …•X Ñ i A| l \ ä . ($i = 2$ t tt $A = \{0,1,2,4,5\}$)
- AÐ • \ …• ´ p …• i@X p ¬ Á 8 ' © ½ r_0ô ä '@ …• ä > D $\mathcal{N}_i(r_0)$Ð ¥ \ ä . ($i = 2$t t $\mathcal{N}_2(r_0) = \{1\}$)

\ …• ù 9 X @Ð ì h …• @X p ¬Ì D D P X 0 L 8 Ð typical caseÐ Ä ° É @ $O(N)$t ä .

3.3 GPU를 \ ©\ Ñ 렬 계°

GPU” ¨ à …•X • Ä ÙÜÐ 1 à ” (parallel update) „ • Ùí Y Ä ° D Ñ , ˜ ¬ X ” p \ T ð ° ¥ X t ä . GPU Ä Ä ° ¥ %D 100| < ¸ \ © X $ t gpuX hardware ' ÙÐ¬Ð \ J @t t D ” X À Ì , D õ ¬ © •X …¥ Ð t ” ä ° ´ $ ´ |t ä . t X Ð ” Nvidia¬ X GPUÐ CUDA (Compute Unified Device Architecture)| ¬ ©t Ñ , Ä ° D ‰X ” p D ” \ \ Œ\ X ô Ì D “D• t t X”) Ý < \ ” $ … ` ƒ t ä [2].

3.3.1 GPUX 구p @ ' 동Ð 리

- GPU” LED ¨ È 0 \ D ` ˆ ä . ¨ È 0 X grid Œ\ $(m,n)$È ä = @t ì ´ 8 ˆ ï , Nvidia¬ X GPU Ð ” ð ° D ‰` ˆ à à X grid Œ\ (m,n) 9 @ (l,m,n)D À ` ˆ ” œ X cuda cores

[2] ¬ t ¸ https://sites.google.com/view/jdnoh/lecturesÐ tutorialÐ ¬ © cuda@ python source code| ä ´ \ Ü ` ˆ ä .

ì ´ 8 ì ´ 8 ˆ ä .

- ø ˜ = ô ü ´ À t¨ È 0 X = @t Œ\ Ð ` ù rgb à 8 | ÙÜÐ œ%X ï t ,cuda cores” • à X ø ¬ Ü Œ\ D 8 p X p h Ä ° D Å ½ < \ ÙÜÐ ‰\ ä .
- SPP …• | cuda coreÐ QÜ ü t „ • Ùí Y Ä ° D Ñ,\ ‰` ˆ ä .

3.3.2 CUDA kernel

cuda kernel@ cuda cores ‰` ' Å D X \ h 9 @ è ô D À m\ ä . 2^{18} (ÐX P ¡ 0 $\boldsymbol{a}, \boldsymbol{b}$X i $\boldsymbol{c} = \boldsymbol{a} + \boldsymbol{b}$D l X $ t ,cuda kernel@ D˜ @ @) Ý < \ X X à

```
__global__ void a_plus_b_equal_c(int *a, int *b, int *c)
{
    unsigned int tid = threadIdx.x + blockIdx.x*blockDim.x;
    c[tid] = a[tid] + b[tid];
}
```

ä LX) Ý < \ 8 œ\ ä .

```
int nBlock = 1024, nThread = 256;
a_plus_b_equal_c<<<nBlock, nThread>>>(a, b, c);
```

^ ¬ ©\ D | ¬ ©X ì $ …D t ´ ô • .

- <<<1024, 256>>>" 1024 × 256 X = @ ø ¬ Ü| Ä Á ¨ È 0 | Ý 1 X | " À Ü ´ ä . (1 grid = 1024 blocks, 1 block = 256 threads)
- cuda kernelt 8 œ t = @ (cuda core)@ • à X ø ¬ Ü Œ\ D ¬ Ð $ \ ) Ý < \ À X t À ' Å D ‰\ ä . (threadIdx.x = 0, ..., 255, blockIdx.x = 0, ..., 1023, blockDim.x = 256)
- blockDim.x( ] \ Ð ì h ð Ü X /)" **32**X 0 \ !

3.4 CUDA를 \ ©\ „ • 동í Y Ñ 렬계° pseudo code

pseudo code

```
# Vicsek_Config.cu or Vicsek_Tseries.cu

initialize()

for t = 0, ..., T
    Xupdate<<<nBlock, nThread>>>()
    linked_cell()
    PolarAngleUpdat<<<nBlock, nThread>>>()
    Vupdata<<nBlock, nThread>>>()
    write_order_parameter()
```

```
        write_config()

    finalize()
```

package

```
    U•  |  vicsek_turorial.tgz • Ð
        Vicsek_Config.cu (configurationD œ%X”  Tx   \ ø¨ )
        Vicsek_Tseries.cu (order parameter ÜÄôD œ%X”  Tx   \ ø¨ )
        VicsekKernel.cu (cuda kernel)
        VicsekModel.cu (class  X )
```

compile and run (CUDA Version 11.6)

```
    nvcc -O2 Vicsek_Config.cu -o Vicsek_Config.exe -lm -lcurand_static -lculibos
        --extended-lambda

    Vicsek_Config.exe {lx} {ly} {rho} {v0} {eta} {seed} {tmax} {ic=gas or liq}
    =>  | œ%Vicsek_Config_from_{ic}_state_Lx{lx}Ly{ly}Rho{rho}Eta{eta}V{v0}.dat

    Vicsek_Tseries.exe {lx} {ly} {rho} {v0} {eta} {seed} {tmax} {ic=gas or liq}
    =>  | œ%Vicsek_Tseries_from_{ic}_state_Lx{lx}Ly{ly}Rho{rho}Eta{eta}V{v0}.dat
```

3.5 Python< 로 ` 니메t X

PythonX matplotlib.pyplot package| \ ©X ì Vicsek ¨ X Ùí Y D animation< \ U x ` ˆ ä . PythonX ¥ @€ „ Ì \ ð 1 Ð ˆ À Ì , loop Ä ° t À Å X Œ • ¬ ä . t | t ° X ” ì ì À)• tˆ À Ì , D • ” u ì loop| C/C++\ ' 1 X à t | ô | X à | t ì ¬ \ À X \ Ä pythonÐ ˆ ì ð ”)• D ¬ © X à ˆ ä .

- package: U • | `VicsekPython.pgz` • Ð

  `anim.py`, `model.py`: Vicsek ¨ ü ` È T t X

  `sub_local_field.c`: ...•X velocity angleD Å p t ¸ X ” Ä ° D ôù X ” C subroutine

  `SConstruct`: C \ ø ¨ D ô | X ì | t ì ¬ \ Ì Ü ” p D ” \ ¤ l ½ ¸ |

  "scons" software toolD $ X \ Ä , `scons` ...9 ´ | ...%X t SConstruct ¤ l ½ ¸ |t À Ü X ” \ `sub_local_field.c` | ô | \ Ä | t ì ¬ Ý 1 t ä .

- ä ‰ `python3 anim.py`

3.6 8 고 • 료

- CUDA õ Ý H ˜ t À https://developer.nvidia.com/cuda-zone

  CUDA quick start guide, tutorial, CUDA C/C++ programming guide, ...

- Thrust https://developer.nvidia.com/thrust

GPUĐ ©\ utilitiesX ¨ L : `sort_by_key, fill, reduce, ...`

- CuPy H˜ t À https://cupy.dev/

CUDA with python

4

t ð 구)•

…• 0 X ¨ Ð \ 1 xt t | t Ä • Ä DÜÐ \ ¥t ` D õ € t ô • . ¥t ` @ scalar field x Ä $\rho(\boldsymbol{r},t) = \sum_i \delta(\boldsymbol{r}-\boldsymbol{r}_i(t))$@ vector fieldx polarization $\boldsymbol{p}(\boldsymbol{r},t) = \frac{1}{\rho(\boldsymbol{r},t)}\sum_i \frac{\boldsymbol{v}_i(t)}{|\boldsymbol{v}_i(t)|}\delta(\boldsymbol{r}-\boldsymbol{r}_i(t))$, 9 @ ´ ÙÉ Ä (magnetic systemÐ D t • T Ä| mX 0 Ä \ ä) $\boldsymbol{m} = \rho\boldsymbol{p}$ Ð \ ð •) ÝD ÄX ” f < \ Ü' \ ä .

4.1 Boltzmann) Ý

ü Ì) Ý @ …• ÄX 1 ÈD one-particle distribution function

$$f(\boldsymbol{r},\theta,t) = \left\langle \sum_{i=1}^{N} \delta(\boldsymbol{r}-\boldsymbol{r}_i(t))\delta(\theta-\theta_i(t)) \right\rangle \quad (\boldsymbol{r}_i, \theta_i : \text{position and polar angle of the } i\text{th ptl.}) \tag{4.1}$$

D µ t 0 \ ä [BDG09]. $\langle()\rangle$@ U` x ´ Ù ½\ Ð \ ÉàDX ø\ ä . f h ”

$$\frac{1}{V}\int_V d\boldsymbol{r}\int_{-\pi}^{\pi} d\theta f(\boldsymbol{r},\theta,t) = \frac{N}{V} = \rho_0 \tag{4.2}$$

D Ì q \ ä (normalization p t).

4.1.1 Time evolution

δtX ÙH fh X À T $\delta f = f(\boldsymbol{r},\theta,t+\delta t) - f(\boldsymbol{r},\theta,t)$| " t ô • .

- self-propulsion: $\boldsymbol{r} \to \boldsymbol{r} + v_0 \boldsymbol{n}_\theta \delta t$

$$\left.\frac{\delta f}{\delta t}\right|_{s.p.} = \frac{f(\boldsymbol{r} - v_0\boldsymbol{n}_\theta\delta t,\theta,t) - f(\boldsymbol{r},\theta,t)}{\delta t} = -v_0 \boldsymbol{n}_\theta \cdot \boldsymbol{\nabla} f \ . \tag{4.3}$$

- $\lambda\delta t$X U` \ | ´ ˜ " ´ Ù ÄX 4 ' x U° (self diffusion): $\theta \xrightarrow{\lambda\delta t} \theta + \zeta$ t à $\zeta$X U` „ ì h " $P_\eta(\zeta)$t ä (É à @ 0, „ ° @ η^2).

$$\left.\frac{\delta f}{\delta t}\right|_{s.d.} = -\lambda f(\boldsymbol{r},\theta,t) + \lambda \int_{-\pi}^{\pi} d\theta' \int d\zeta f(\boldsymbol{r},\theta',t) P_\eta(\zeta) \delta_{\text{mod } 2\pi}(\theta - (\theta' + \zeta)) \tag{4.4}$$

$$= \lambda \left[-f(\boldsymbol{r},\theta,t) + \int_{-\pi}^{\pi} d\theta' f(\boldsymbol{r},\theta',t) P_\eta(\theta - \theta') \right] \tag{4.5}$$

- binary collision: Ä ®ä t K t ÁX …• ÙÜÐ ©Ì Xì Á8 ' ©X" ¬t D 4Ü` ˆ ä.´ Ù Ä (θ_1,θ_2)x P …• ©Ì t • Ä , Á8 ' ©D ª Èäà X• .• Ä , ÐÄ P_η „ ì | 0t " ¡Lt ' ©\ ät …•X ´ Ù Ä"

$$\theta_1 \xrightarrow{\delta t K(\theta_2 - \theta_1)} \theta_1 + H(\theta_2 - \theta_1) + \zeta, \tag{4.6}$$

$$\theta_2 \xrightarrow{\delta t K(\theta_2 - \theta_1)} \theta_2 - H(\theta_2 - \theta_1) + \zeta'. \tag{4.7}$$

t à $H(\phi = \theta_2 - \theta_1)$" D \ • Ä , t| ´ ¬ D L X ° € Ät ä . Vicsek-typeX ½° Ð"

$$H(\phi) = \frac{\phi}{2}. \tag{4.8}$$

$K(\phi)$" Ä (t ϕx P ...•X total scattering rate| X ø \ ä . ...•X Á 8 ' © p ¬ r_0t à Á • Ä X l 0 $v_0|\boldsymbol{n}_\phi - \boldsymbol{n}_0| = 2v_0 \sin|\phi/2|$„D à $ X t ä LD » D ˆ ä .

$$K(\phi) = 4r_0v_0K_0(\phi) \quad \left(K_0(\phi) := \sin\left|\frac{\phi}{2}\right|\right) \tag{4.9}$$

0 | ,

$$\left.\frac{\delta f}{\delta t}\right|_{coll} = -4r_0v_0 \int d\theta' K_0(\theta - \theta') f_2(\boldsymbol{r}, \theta; \boldsymbol{r}, \theta') \tag{4.10}$$

$$+ 4r_0v_0 \iiint d\theta_1 d\theta_2 d\zeta K_0(\theta_2 - \theta_1) f_2(\boldsymbol{r}, \theta_1; \boldsymbol{r}, \theta_2) P_\eta(\zeta) \delta_{2\pi}(\theta - (\theta_1 + H(\theta_2 - \theta_1) + \zeta)) \tag{4.11}$$

$$= -4r_0v_0 \int d\theta' K_0(\theta - \theta') f_2(\boldsymbol{r}, \theta; \boldsymbol{r}, \theta') \tag{4.12}$$

$$+ 4r_0v_0 \iint d\theta_1 d\theta_2 K(\theta_2 - \theta_1) f_2(\boldsymbol{r}, \theta_1; \boldsymbol{r}, \theta_2) P_\eta(\theta - \theta_1 - H(\theta_2 - \theta_1)). \tag{4.13}$$

X Ý @ two-particles distribution function $f_2(\boldsymbol{r}_1, \theta_1; \boldsymbol{r}_2, \theta_2; t)$D ì hX à ˆ ä . | < \ n-particles distribution functionX ´ Ù) Ý @ $(n+1)$-particles distribution functionD ì hX à ˆ ´ , ´) Ý @ 4 \ ˆ Î @„ ì h ä t Ä 5 < \ ° i Bogoliubov–Born–Green–Kirkwood–Yvon (BBGKY) hierarchy l p | "ä . t œ D ¨t X 0 t É à ¥ ü ¬ 9 @ **molecular chaos** D DÝ X • .

$$f_2(\boldsymbol{r}_1, \theta_1; \boldsymbol{r}_2, \theta_2; t) = f(\boldsymbol{r}_1, \theta_1, t) f(\boldsymbol{r}_2, \theta_2, t) \tag{4.14}$$

Ä ®à …• -…• Á Ä| 4Ü` ˆ ä” D µ t » @ Boltzmann) Ý @ D˜ @ ä .

$$\partial_t f(\boldsymbol{r},\theta,t) + v_0 \boldsymbol{n}_\theta \cdot \boldsymbol{\nabla} f(\boldsymbol{r},\theta,t) = \lambda \left[-f(\boldsymbol{r},\theta,t) + \int_{-\pi}^{\pi} d\theta' f(\boldsymbol{r},\theta',t) P_\eta(\theta-\theta') \right] - 4r_0 v_0 \left[f(\boldsymbol{r},\theta,t) \int d\theta' K_0(\theta-\theta') f(\boldsymbol{r},\theta',t) + \iint d\theta_1 d\theta_2 K_0(\theta_2-\theta_1) f(\boldsymbol{r},\theta_1,t) f(\boldsymbol{r},\theta_2,t)) P_\eta(\theta-\theta_1-H(\theta_2-\theta_1)) \right]. \tag{4.15}$$

™Ä À X $t \to t/\lambda$, $\boldsymbol{r} \to \frac{v_0}{\lambda}\boldsymbol{r}$, $f \to \rho_0 f$ D µ t Ü ü À @ Ä| 4 (Ð À \ \ ÜXt Ý (4.15)Ð $\lambda = v_0 = 1$\ “ D ˆ à Ý (4.2)Ð Ä $\rho_0 = 1$\ “ D ˆ ä . 4 (Ð) Ý Ð Ý (4.9)X total scattering rate h ” $K(\phi) = 2\pi\kappa K_0(\phi)$t à , • Ä , Á 8 ‘ ©X 8 0 ” 4 (Ð ° i Á κ\ t Ä ä .

$$\kappa = \frac{2r_0 v_0 \rho_0}{\pi\lambda} \tag{4.16}$$

4.1.2 Angular Fourier mode expansion

®@ ÄÐ É à ¥ ü ¬| è ˆ L ÐÄ ˆ l X à Boltzmann) Ý @ ì ˆ õ ¡ X ä . t ` x ü D t one-particle distribution functionX moments, 9 @ Fourier modes| à $ X • .

$$\hat{f}_k(\boldsymbol{r},t) = \int_{-\pi}^{\pi} d\theta f(\boldsymbol{r},\theta,t) e^{ik\theta} \quad \Leftrightarrow \quad f(\boldsymbol{r},\theta,t) = \frac{1}{2\pi} \sum_{k=-\infty}^{\infty} \hat{f}_k(\boldsymbol{r},t) e^{-ik\theta} \tag{4.17}$$

Fourier modesX ¹ 1 D ¬ t ô • .

- $\hat{f}_{-k}(\boldsymbol{r},t) = \hat{f}_k^*(\boldsymbol{r},t)$

- $\hat{f}_0(\boldsymbol{r}, t) = \rho(\boldsymbol{r}, t)$: ...• Ä
- $\rho \boldsymbol{p}(\boldsymbol{r}, t) = \begin{pmatrix} \mathrm{Re}\ \hat{f}_1 \\ \mathrm{Im}\ \hat{f}_1 \end{pmatrix}$: ´ ÙÉ Ä (...• Ä × polarization) = local flocking order parameter
- $\rho \boldsymbol{Q} = \frac{1}{2} \begin{pmatrix} \mathrm{Re}\ \hat{f}_2 & \mathrm{Im}\ \hat{f}_2 \\ \mathrm{Im}\ \hat{f}_2 & -\mathrm{Re}\ \hat{f}_2 \end{pmatrix}$: nematic tensorial field (´ ÙÉ Ä X Dñ) 1)

Fourier Ð \ convolution ¬ ($C(\theta) = \int d\theta' A(\theta - \theta') B(\theta')$X Fourier modes" $\hat{C}_k = \hat{A}_k \hat{B}_k$)| \ ©X t θ õ Ð X Boltzmann) Ý (4.15)D Fourier ¨ Ü ¬ tX ° i) Ý < \ • } Œ À ˆ ä [1].

$$\partial_t f_k(\boldsymbol{r}, t) + \frac{1}{2}(\partial_x + i\partial_y) f_{k-1} + \frac{1}{2}(\partial_x - i\partial_y) f_{k+1} = -(1 - P_k) f_k + \kappa \sum_{l=-\infty}^{\infty} \mathcal{J}_{kl}\ f_{k-l}(\boldsymbol{r}, t) f_l(\boldsymbol{r}, t), \text{where} \tag{4.18}$$

$$P_k = \int d\zeta P_\eta(\zeta) e^{-ik\zeta} = e^{-k^2\eta^2/2}, \mathcal{J}_{kl} = P_k I_{k/2-l} - I_l, I_u = \int_{-\pi}^{\pi} d\theta K_0(\theta) e^{iu\theta} = \begin{cases} \frac{4}{1-4u^2}, & u : \text{integer} \\ \frac{4}{1+2u \sin u\pi}, & u : \text{half-integer} \end{cases} \tag{4.19}$$

4.1.3 균| \ 4 È Á Ü

à | \ 4 È Á Ü 9 @ 0 ´ Á Ü Ð t ù X " Á Ü

$$f_k(\boldsymbol{r}, t) = f_{G,k} := \delta_{k0} \tag{4.20}$$

---

[1] $ t X ì À ÆD ½° Fourier modes| X ø X " ˆ0 8 | Ý µ X ä .

” ü Ì) Ý (4.18)X Ô\ ÁÁ Ü t t ä . t t à | \ - Ù

$$f_k(\boldsymbol{r},t) = f_{G,k} + \epsilon_k(t) \quad (|\epsilon_k| \ll 1) \tag{4.21}$$

Ð t H \ À ´ ´ ô • (linear stability analysis). ü ¬ Ð $k \neq 0$x - Ù m@ ´ Ù) Ý

$$\dot{\epsilon}_k = \mu_k \epsilon_k + O(\epsilon^2) \quad (\mu_k := -(1-P_k)\kappa(\mathcal{J}_{k0} + \mathcal{J}_{kk})) \tag{4.22}$$

D 0 x ä . ¨ à Fourier modes \ Å ½ „D L ˆ ä . Order parameterÐ t ù X ” $k = 1$ ¨ Ü X H p t $\mu_1 = -(1 + 8\kappa/3) + (1 + 4\kappa)P_1 < 0$< \ € 0 à | \ 4 È Á Ü ˆ H t À ” ¡L 8 0 X … Ä D l ` ˆ ä .

$$\eta_c(\kappa) = \sqrt{-2\log\left(\frac{1+8\kappa/3}{1+4\kappa}\right)} \tag{4.23}$$

4.1.4 균| \ flocking ordered state

’ @ Ä 9 @ ‘@ ¡L ($\eta < \eta_c(\kappa)$) íÐ à | \ 0 ´ Á Ü ” ˆ H t Ä ä . D ˜ X è Ä | D p à | \ 0 ´ Á Ü D Ì íÐ X Á É ø ¼D l t ô • .

1. à | \ ($\partial_x = \partial_y = 0$) a ´ Á Ü Ð t ù X ” ÁÁ Ü ($\partial_t = 0$) t $f_k(\boldsymbol{r},t) = f_{L,k} \neq 0$| ð ½) Ý

$$(1-P_k) f_{L,l} = \kappa \sum_l \mathcal{J}_{kl} f_{L,k-l} f_{L,l} \tag{4.24}$$

D € ´ l \ ä . X < \ ” x ¬ Ð ¨ Ü | $|k| < k_c$x í < \ \\ Ä iteration)• < \ l ` ˆ ä .

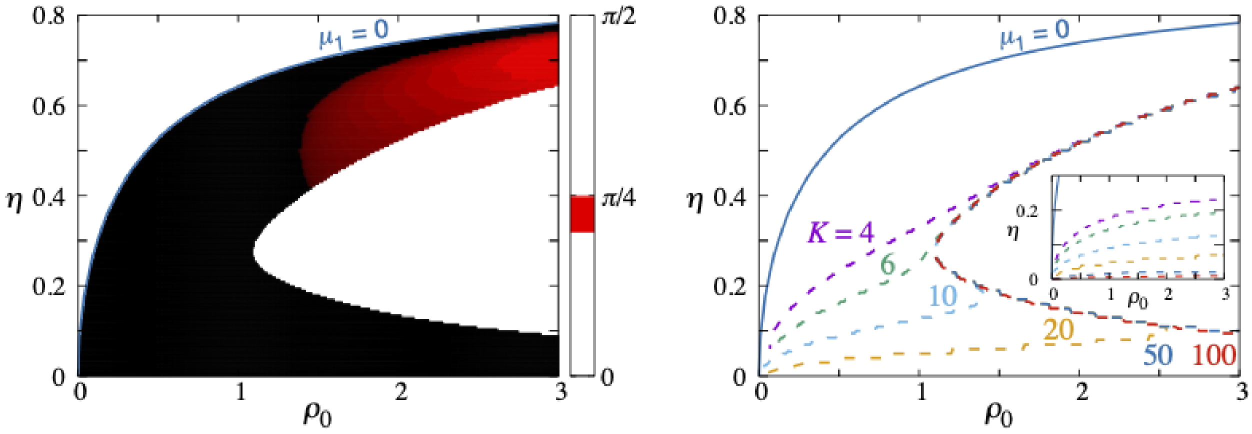

Figure 4.1: Boltzmann) Ý X Á É ø ¼ ([Mah18]Ð Ì h . ø ¼X ρ_0@ ø 8 X κ ¬ t Ð" $\rho_0 = \pi\kappa$X Ä ˆ ä .)

2. à | \ a ´ Á Ü $f_{L,k}$Ð wave vector $\boldsymbol{q} = (q_x, q_y)$x ˆ à x \ É t " Ù X linear stability| p ¬ \ ä .

$$f_k(\boldsymbol{r}, t) = f_{L,k} + \delta f_{k,\boldsymbol{q}}(t) e^{i\boldsymbol{q}\cdot\boldsymbol{r}} \tag{4.25}$$

ü ¬ Ð " Ù X ´ Ù) Ý @

$$\frac{d}{dt}(\delta f_{k,\boldsymbol{q}}) = \mathcal{M}(\boldsymbol{q})_{kl}(\delta f_{l,\boldsymbol{q}}) \tag{4.26}$$

t à , H 1 D ° X " ‰, @

$$\mathcal{M}(\boldsymbol{q})_{k,l} = -(1 - P_k)\delta_{kl}(1 - P_k) - \frac{i}{2}\left((q_x + iq_y)\delta_{k,l+1} + (q_x - iq_y)\delta_{k,l-1}\right) + \kappa\left(\mathcal{J}_{k,l} + \mathcal{J}_{k,k-l}\right) f_{L,k-l} \tag{4.27}$$

t ä .

3. X $\boldsymbol{q}$Ð H 1 ‰, $\mathcal{M}(\boldsymbol{q})$X à X| l Xà,ä€ ¸ ' X D " à X t ¬ X" À p ¬ \ ä.¨ à $\boldsymbol{q}$Ð ¨ à à XX ä ¸ L x íÐ ,à| \ a´ ÁÜ H x t ä.Ì } ,ä ¸ ' x à X X˜ | Ä t ¬ \ ät ,ø íÐ à| \ a´ ÁÜ" ˆ H Xä.

ø ¼ 4.1Ð ÉT\ ` t Ä €„ @¹ \ $\boldsymbol{q}$X " ÙÐ Xt à| \ a´ ÁÜ ˆ H t À" ít ä. ¥ ˆ H 1 t ' @" ÙX wave vector" $\boldsymbol{q} \neq 0$„t L ä [Mah18]. ÉTt ` t Ä íÐ ÄX…• polarization X „ ì ˆ à| h D ´ ì Xà ˆ ä. t íÐ Boltzmann) Ý (4.15)Ð X „ Xt ¡<\ ˜ ´ ì ì X band Ä‰X" f D Ux ` ˆ ä [Mah18]. t Á<\ ° ¬ " Boltzmann) Ý<\ €0 à| \ 0´ ÁÜ (disordered phase), à| \ a´ ÁÜ (flocking phase), ˆ à| \ õt ÁÜ (bands phase)\ l 1 ÁÉ ø ¼ (4.1)D »È ä. Vicsek ¨ X ÁÉ ø ¼ (2.2) ¬ tX ¬ 1 ü (t D Uxt ô8 €ä.

4.1.5 Hydrodynamic equation

Boltzmann) Ý<\ €0 ÁÉ ø ¼X 1 x ¹ 1 D t tˆ <˜ ,ì t X ü)• Ð À˜ XŒX t Xà ˆ ´ Á t TäÈ˜ Dt tX 0 ´ 5ä.t x ü D t €T ü \ D Ä…X•.ˆ à| \ õt ÁÜÐ 0´ ÁÜ ½ ½Ä (Ý (4.23))<\ ä] $f_{k\geqslant 1}(\boldsymbol{r},t)$X l 0 ´ <\ ' DÈ f t ä. \ ½ Ä <\ ä] ÄX Dñ) 1 t ´ ä f t ä.t ì \ 0 | \ Xì ´ Fourier modes ´ p $k=0$ ¨ Ü (…• Ä), $k=1$ ¨ Ü (polarlization)Ì ¨ 0 à ˜ 8 À ¨ Üä D ¨ ü <\ p \ hydrodyanmic) ÝD Ät ô• [BDG09]. $f_0 = \rho$, $f_1 = \rho(p_x + ip_y)$„D Á0 X•.

Ý (4.18)Ð $k = 0,1,2$| …Xì hydrodynamic field ρ, $\boldsymbol{p}$@ leading correction termÐ \ ´ Ù) ÝD l t ô•.

- particle density ($k = 0$)

$$\partial_t \rho + \frac{\partial_x}{2}(f_{-1} + f_1) + \frac{i\partial_y}{2}(f_{-1} - f_1) = 0 \quad \Rightarrow \quad \partial_t \rho + \nabla \cdot (\rho \boldsymbol{p}) = 0. \tag{4.28}$$

- polarization ($k = 1$)

$$\partial_t f_1 + \frac{\partial_x}{2}(f_0 + f_2) + \frac{i\partial_y}{2}(f_0 - f_2) = -(1 - P_1) f_1 + \kappa(\mathcal{J}_{1,0} + \mathcal{J}_{1,1}) f_0 f_1 + \kappa(\mathcal{J}_{1,2} + \mathcal{J}_{1,-1}) f_2 f_{-1} + O(f_{|k|\geqslant 3}) \tag{4.29}$$

- nematic order parameter ($k = 2$)

$$\partial_t f_2 + \frac{\partial_x + i\partial_y}{2} f_1 = -(1 - P_2) f_2 + \kappa \left(\mathcal{J}_{20} f_2 f_0 + \mathcal{J}_{2,1} f_1^2 + \mathcal{J}_{22} f_0 f_2 \right) + O(f_{|k|\geqslant 3}) \tag{4.30}$$

f_2” hydrodynamic fieldsô ä time scalet ç D mÁ quasi-steady stateÐ ü t ˆ ä à X t Ý (4.30)Ð $\partial_t f_2$m D 0< \ “ D ˆ à , f_2| f_0ü f_1h \ l ` ˆ ä . t Œ l \ $f_2$| Ý (4.29)Ð …X à ¬ X t …• Ä @ ´ Ù É Ä $\boldsymbol{w} = \rho \boldsymbol{p}$\ t Ä ë Œ ´ Ù ) Ý D » D ˆ ä . U \ 4 X ´ Ù ) Ý @ 8 à 8 Ì ([BDG09] X Ý (27-32))Ð U x X 0 \ X à , ¥ ” \ í ` D X ” mÌ ´ ´ ô • .

$$\partial_t \boldsymbol{w} + \gamma(\boldsymbol{w} \cdot \nabla)\boldsymbol{w} = \left\{ \mu(\rho) - \xi(\rho)\boldsymbol{w}^2 \right\} \boldsymbol{w} + \text{additional terms} \tag{4.31}$$

‰@ É < \ \ Ü \ m @ vector order parameter| ” Ä X Landau-Ginzburg t ` Ð ñ ¥ X ” mt ä . $\xi > 0$ x Landau-Ginzburg t ` Ð , reduced temperature í ` D ôù X ” $\mu$ t L Ð ‘ \ À h Ð 0 | Ä ” disordered phase ($\boldsymbol{w} = 0$)@ ordered phase ($\boldsymbol{w} \neq 0$) ¬ t Ð Á t | ª ”ä . ô É Ä X Landau-Ginzburg t ` ü X (t @ effective reduced temperature μ local densityÐ X t \ ä” t ä . ‰,

$$\mu(\rho(\boldsymbol{r})) = 4\kappa\frac{\rho(\boldsymbol{r})}{\rho_0}\left(e^{-\eta^2/2} - \frac{2}{3}\right) - \left(1 - e^{-\eta^2/2}\right). \tag{4.32}$$

…•X Ä Ð ‘@ ” Ùt Ý X t $\rho(\boldsymbol{r}) > \rho_0$x í ü $\rho(\boldsymbol{r}) < \rho_0$x í t ˜ X Œ ä . Ä ’ D Ä íÐ ” μ t ‘ ´ …• ä t Ñ è < \ \ ) ¥ < \ À Á t à 0 | …•X local density” T ± T ’ D Ä ä . t Ð X íÐ ” μ t L ü ´ …• ä t È l ¡t \ À Á t p ü À Ð a ´ local density” T ± T ® D Ä ä . …• Ä Ð X t X ” effective reduced temperature Vicsek-type ¨ Ð ˜ À ˜ ” bandsÐ X \ microphase separationX T t È ˜ „D L ˆ ä . Hydrodynamic equationÐ \ • 8 X à Ä \ Ä ° @ [BDG09]D 8 à X | .

4.2 Smoluchowski) Ý

Bolzmann) Ý t coarse-grain Vicsek-type ¨ X ¥) Ý Ð i\ t Ð , Ý (3.3)ü @ ð • Ü ´ Ù) Ý D 0 t ” ABP 0 ¨ X ¥) Ý @ Smoluchowski) Ý t iX ä . t)• @ Langevin Ù í Y D 0 t ” ä ´ Ä X ¥) Ý D Ä \ DeanX t ` [Dea99]D ABP ¨ Ð © X ” ƒ t ä [GRBSG14]. ä ´ Ä X U ` Ä h Ð œ t í Ý molecular chaos D Ä …X t , one-particle distribution functiont Ì q X ” Smoluchowski) Ý D Ä ` ˆ ä . Boltzmann) Ý ü X ì ¬ Smoluchowski) Ý @ multiplicative stochastic noisem D ì hX à ˆ ä .

5

망

5.1 Beyond mean field theory

Boltzmann) Ý ü Smoluchowski) Ý , ø ¬ à ø \ € 0 Ä hydrodynamic) Ý ä @ ¨ P *molecular chaos*| \ É à ¥ t ` t ä . É à ¥ t ` < \ Vicsek-type ¨ Ð Ý X " 4 È 0 ´ Á , ¼ À L a ´ Á , õ t Á t t ¬ " Á É ø ¼ , ø ¬ à Á Ü Ð X < 1 D t t` ˆ ä . Á É ø ¼ Ð Ì t D È | „ Ä Á X ô ¸ 1 D t " É à ¥ t ` D ð ´ " t ` x ü t D " X ä .

\ ´ ´ " Á 8 ' © D P X X " ¥ Ù …•X Á „ ¬ Á (MIPS, motility-induced phase separation)Ä hydrodynamic) Ý D µ t \ ˆ ð l à ˆ ä . ô É Ä Ð | ´ ˜ " 0 ´ -a ´ Á „ ¬ Á @ model BX " ü \ „ X " ¤ | | ¥) Ý < \ 0 ä [HH77].

$$
\begin{aligned}
\partial_t \phi &= -\boldsymbol{\nabla} \cdot \left(\boldsymbol{J} + \sqrt{2DM}\boldsymbol{\Lambda} \right) \\
\boldsymbol{J} &= -M \boldsymbol{\nabla} \mu_{eq} = -M \boldsymbol{\nabla} \frac{\delta F}{\delta \phi} \quad \text{with } F[\phi] = \int \left\{ \frac{a}{2}\phi^2 + \frac{b}{4}\phi^4 + \frac{K}{2}|\boldsymbol{\nabla}\phi|^2 \right\}
\end{aligned}
\tag{5.1}
$$

X Ý Ð • Ð À m< \ € 0 Ä À J " mD " h < \ h ô É t ` D ¥ Ù < È Ä \ U ¥ ` ˆ ä .

| ä ´

$$\boldsymbol{J}/M = -\boldsymbol{\nabla}\left[\frac{\partial F}{\partial F} + \lambda|\boldsymbol{\nabla}\phi|^2\right] + \zeta(\nabla^2\phi)\boldsymbol{\nabla}\phi \tag{5.2}$$

\ U¥\ t ` x active model B+ (AMB+) ˆ ä [TNC18]. X ÝÐ ¡L mD 0<\ " @Éà¥t ` Ì <\ Ä ä° eø\ ´ Á„ ¬ ÁD ôxä.Éà¥t ` D ´ ¡L mX ¨ ü ¨ P à$ stochastic field theory Ð \ ðl D" \ Ü t ä.

5.2 Discrete symmetry flocking

Vicsek-type ABP ¨ X ´ € • ÄÐ t ùX" •Ä)¥ Ä θ" ð• ÀX $(\theta \to \theta + \phi)$Ð t m t ä. ð• m1 D DT\ ˆ ð• ÀX m1 D "¥ Ù<ÈÄX ÑèpÙ@t ` <\ ä° eø\ ´ ðl ü t ä. •Ä)¥¡ 0 $\boldsymbol{n} = (\cos\theta, \sin\theta)$X)¥ Ä p X ˆ ð• x

$$\theta = \frac{2\pi s}{p}, \quad (s = 0, 1, \cdots, p-1) \tag{5.3}$$

<\ \ active p-state clock modelD Ý t ô• [CMR22, SCTT22]. Vicsek ¨ @ $p = \infty$x ù\ Ð t ùXp, ¥ è\ $p = 2$x ½° " active Ising model (AIM)Ð t ù\ ä [ST13].

\ t ` x eø| ´ AIM@ flocking Á t 0´ -a´ Á t @ @ Á„D U½X" p ° x 0ì | ˆ ä [SCT15]. øì ˜ ,\ üÐ ÈmŒ \ ðl °ü " ' à ç@Ü ÙHÐ ‰ " X Ü‰´ 0Ð »@°ü @Éà¥t ` 0 D hydrodynamic) ÝÐ »@°ü ¼È˜ è} ` ˆ " À| ì äˆ ôì üàˆ ä [BGR+23, WN24]. AIMX ðl X P„ D èˆ ¬t ô•.

1. AIMX ñ¥< \ flocking Á tX 0´ Á → õt Á → a´ Á tt ` X ½ Èä [SCT15].

2. Droplet excitationt È m Œ ¬ ´ ¥ p ¬ È | " a ´ Á Ü metastable Á Ü | " ƒ t L ä . t \ x t 0 ´ -a ´ Á t t ` X ü p ¬ | L ä [BGR+23].

3. Motility-induced interface pinning (MIIP) Á t È m Œ ¬ È ä . MIIP\ x t ¡LX 8 0 'D L Ä X Á Ü a ´ Á Ü D Ì disordered pinned state ä [WN24].

4. t ƒ t] t D Èä .

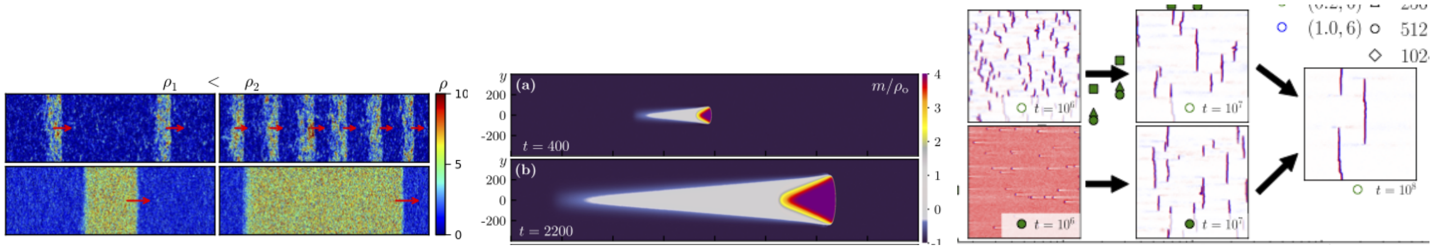

Figure 5.1: Band, droplet, and MIIP in the AIM ([SCT15, BGR+23, WN24]Ð Ì).

5.3 Chirality

Ý < Ä X ä ' 1 @ < ¬ Y • Ð Œ J „ Æt È \ ´ D õ X à ˆ ä . *Paenibacillus vortex* L ¬ D Ñ è @ Ä ´ X ½Ä | 0 | P t " edge current| Ì ä à [LCS+24], molecular motor assayÐ , $ Ä microtublesü [SNS+12] ¸ ¨ \ À Á t " ´ Ù L ¬ D *Serratia marcescens*@ p Ü x I 0 ($O(1mm)$)X vortex array| Ý 1 X à [SNS+12, XW24], Ä ' @ *E. coli*" \ X ´ Ù D Ù 0 T t Ð´ Ù Ù D Ì à ä [CLS+17]. t ä Ä | t è " …• ä @ chirality| à ˆ ´ , • Ä , Á 8 ' © t Vicsek-type ¨ ô ä ä ' \ Ù Á D ô x ä .

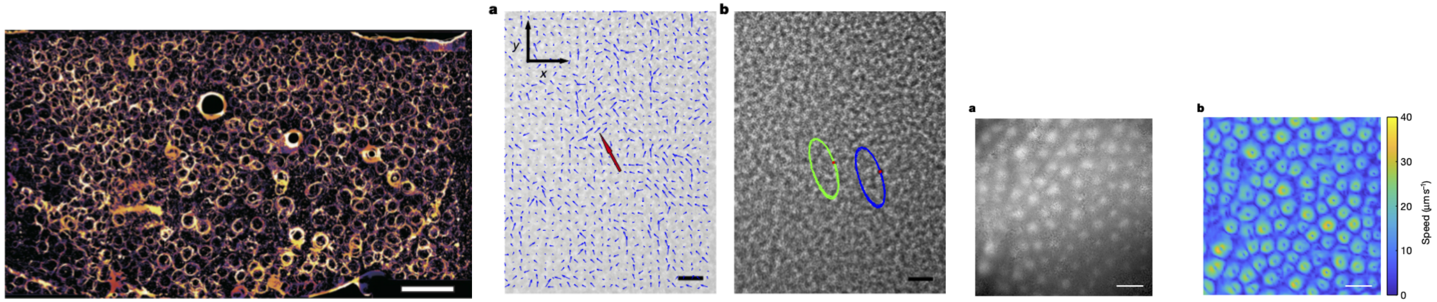

Figure 5.2: vortices in bacteria ([SNS+12, CLS+17, XW24]Ð Ì).

Vortex array (4 D $ …X 0 t Sumino ñ @ …Ü x chirality| ì h\ ¨ Ä | Ü X ä [SNS+12]

$$
\begin{aligned}
\boldsymbol{r}_i &= v_0 \boldsymbol{n}_\theta \\
\dot{\theta}_i &= \omega_i + \frac{\alpha}{|\mathcal{N}_i(r_0)|} \sum_{j \in \mathcal{N}_i(r_0)} \sin(\theta_j - \theta_i) \\
\dot{\omega}_i &= -\frac{1}{\tau}(\omega_i - \omega_0) + \xi_i(t)
\end{aligned}
\tag{5.4}
$$

Chirality| …Ü < \ Ä …ˆ 0 L 8 Ð t ¨ t vortex array (4 D ô ì ü " *f* @ € | ´ |t D Èä . \ ¸ Xu

@ Wu" ø ä X ä Ø °ü | ä LX ¨ < \ ¬ ` ˆ ä à ô à X ä :

$$
\begin{aligned}
\boldsymbol{r}_i &= v_0 \mu_i f_i \boldsymbol{n}_\theta + \sqrt{2D_r}\boldsymbol{xi}_{r,i} \\
\dot{\theta}_i &= \omega_i + \frac{k_\theta}{|\mathcal{N}_i(r_0)|}\sum_{j\in\mathcal{N}_i(r_0)} \sin(\theta_j - \theta_i) + \sqrt{2D_\theta}\xi_{\theta,i} \\
\dot{\omega}_i &= -\frac{\omega_i}{\tau} + \frac{k_\omega}{|\mathcal{N}_i(r_0)|}\sum_{j\in\mathcal{N}_i(r_0)} (\omega_j - \omega_i) + \mathrm{sign}(\omega_i) e^{-|\omega_i|\omega_0} + \sqrt{2D_\omega}\xi_{\omega,i}(t)
\end{aligned}
\tag{5.5}
$$

$\omega \leftrightarrow -\omega$X m1 t À à …Ü x chirality| Ä …X À JX L Ð Ä vortex cellt I ä" ƒ @ Á 8 ' © Ð X t $\omega \leftrightarrow -\omega$X m1 t • < \ • 4 È LD X ø \ ä . Chiral active …•X pattern formation@ e ø \ ´ ð I ü ƒ t ä .

5.4 Multi-species system

ì ì …X ¥ Ù …• < i Ä " active matter ð I X È \ ´ ¥D ô à ˆ ä . A, B P …< \ t è ´ Ä Ä Ð …• ¬ tX • Ä , Á 8 ' © X •1 D 2×2‰, $J_{\alpha\beta}$\ ˜ À ´ • $(\alpha, \beta = A, B)$.

- Chatterjee@ õ Ù ð I • ä @ $J_{AA} = J_{BB} > 0$ t à $J_{AB} = J_{BA} < 0$x ½° , ‰ @ … …• | ¬ " • Ä | @) ¥ < \ , X à ä x … …• | ¬ ") ¥ < \ , X " ½° | ð I X ä [CMW+23]. P …X …• " antiparallel flocking state@ parallel flocking state| 1 X p \ | 0 ™X $ " Á 8 ' © D \ © 9 @ Œ<X ") Ý < \ Ñ è p Ù D ô x ä .
- $J_{AB} \neq J_{BA}$x ½° P … ¬ tX Á 8 ' © @ nonreciprocal 1 È D < p [FHLV21], ¹ ˆ $J_{AB} \times J_{BA} < 0$

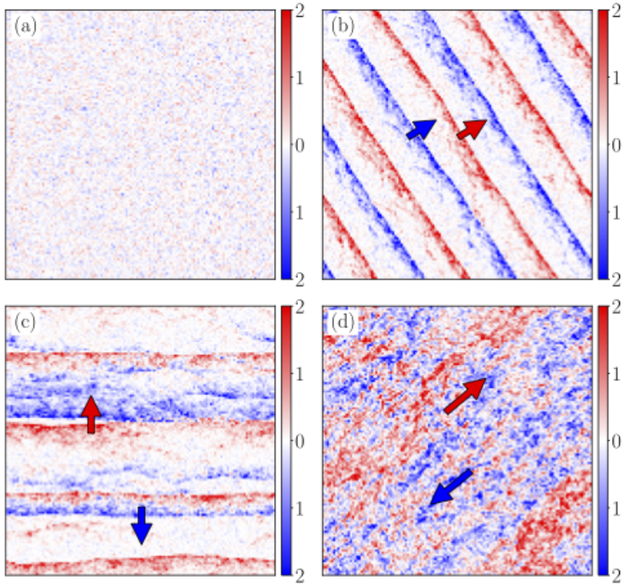

Figure 5.3: Two-species Vicsek ¨ X antiparallel flocking and parallel flocking states ([CMW+23]Đ Ì).

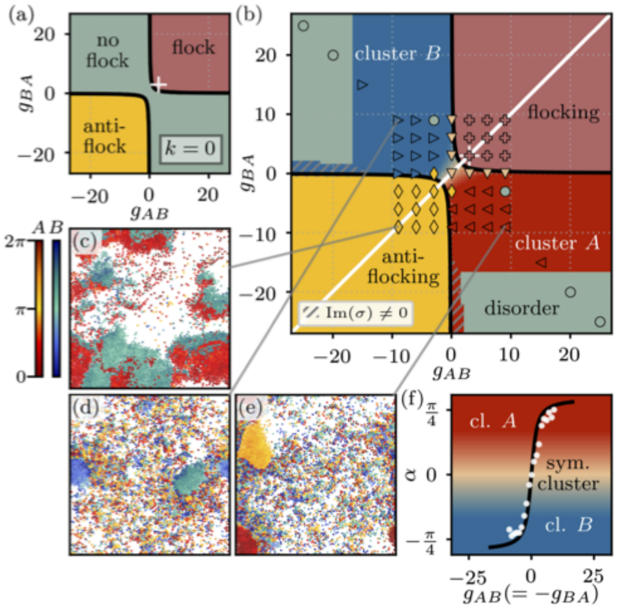

Figure 5.4: Non-reciprocal Vicsek model ([KK24]Ð Ì).

x ½° , …• ä t \ Óà Ó0 p chiral Á Ü 9 @ ˜ ¡ 0 Á Ü, clustering ñ e ø \ ´ Ùí Y Á Ü | ô x ä [MSA^{+}23, MCNR24, KK24].

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