

Phase Transitions and Intermittency in an Aggregation-Fragmentation Model

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Stochastic Model of Diffusion, Aggregation, Fragmentation



•Limiting case of a model of biomolecular movement and processing

•Generalization of well-studied model of aggregationfragmentation in a closed system Shows a transition to a phase with Giant number fluctuations and Intermittency in dynamics $M \propto L$

H. Sachdeva, M. Barma , Madan Rao, Phys. Rev. Lett. (2013)

H. Sachdeva, M. Barma, J. Stat. Phys. (2014)



injection rate *a*

Golgi apparatus



Protein vesicles arrive at one end; leave at other end, after processing

Two scenarios [B Glick et al (1998), E Losev et al (2006), G.H. Patterson et al (2008)]

Vesicular transport: *Biomolecules shuttle between compartments*

<u>Controversy</u> Do biomolecules move singly, or in a bunch?

- 'It is likely that the transport through the Golgi ... involves eleme of both'
- Essentials of Molecular Trafficking (Molecular Biology of the Cell, B Alberts, A Johnson, J Lewis, New Yor Garland : 2002 Cocalized Injection of vesicles containing unprocessed biomolecules
- •**Transport** By chipping of single vesicles, or movement of aggregates



Limiting Cases



Aggregation-Fragmentation Model

Consider the limit of zero interconversion rate : only



- Influx of unit mass with rate a at site 1.
- Diffusion of full stack at rate D or D'. Aggregation o contact.
- **Chipping** of unit mass with symmetric rate w.
- Outflux at site 1 or site L by exit of either the full stack or single particles.



model und

Condensation Phenomena in Closed Systems Zero Range Process (ZRP)

[M R Evans, T Hanney, J Phys A (2005)]

Aggregation-Fragmentation on a Ring

[S N Majumdar, S Krishnamurthy, M Barma, PRL (1998); J Stat Phys (2000)]

The model shows a condensate peak above a critical mass density

Condensate Phase

•Single site mass distribution P(m) shows a power-law + Aggregate peak

•Finite fraction of the mass in the aggregate; akin to Bose-Einstein condensation

Normal Phase



Related work

The mean-field analysis \rightarrow Phase boundary in the w-density plane.



- Phase boundary is exact in all dimensions, despite correlations
 [R. Rajesh and S.N. Majumdar, Phys Rev E (2001)]
- Directed chipping : Condensate lost
 [R.Rajesh and S. Krishnamurthy, Phys Rev E (2002)]
- If $D \sim m^{-\alpha}$, Condensate curbed, but significant effect in finite system [R. Rajesh, D. Das, B. Chakraborty and M. Barma, Phys Rev E (2002)]

Condensation in Open Systems?

- In a closed system with conserved mass, find 'real-space Bose-Einstein condensation'
- The open system has strong mass fluctuations Does condensation occur?

The answer is yes.

The answer is yes. But the condensate is very different in characture from the closed case.



injection rate a

Condensation in the Open System Unbiased Movement (D=D')

Steady state and dynamical properties Very different in the two phases.

Condensate phase •P(m) : Long 'Condensate tail' ... P(M) $\approx A \exp(-M/M_0)$ at

0.06 large M >W>Wc. L=100 0.05 W<Wc 0.1 $M_0 \sim L$ 0.01 0.04 0.001 P(M) 0.0001 •Giant number fluctuations 1e-05 0.03 1e-06 1e-07 ΔM L 1e-08 └─ -2 0.02 >W>Wc, L=200 0.01 Normal (large w) phase •P(m) : Gaussian tail 50 200 250 300 350 400 100

M

Number fluctuations normal

Mass Fluctuations: Size dependence

 $\Delta M \sim L$ in Aggregate Phase $\Delta M \sim L^{2/3}$ at Criticality $\Delta M \sim L^{1/2}$ in Normal Phase





Probability distribution (for p=6 and 0.5, L=100 and 200) Condensate tail $exp(-M/M_0)$ with $M_0 \propto L$

Size dependence of second moment (for w between 2 and 6)

Total mass M: Dynamics





Condensate Phase

Extreme Fluctuations in time

Intermittent, not self-similar

Normal Phase

Fluctuations are self-similar

Self-similarity vs. Intermittency

Self-similarity: $\Delta M(t) = M(t) - M(0)$ has same statistical properties for all t

Intermittency: ΔM(t) depends strongly on t [Distribution of M(t) is heavy-tailed: extreme events dominate]

Define structure functions in time: $u_n(t) = \langle (M(t) - M(0))^n \rangle$ [Analogous to structure functions of velocity field in fluid turbulence]

Self-similar signal: $u_n(t) \alpha t^{\gamma n}$ as $t / \tau \rightarrow 0$ [τ is the lifetime of the largest structures]

Intermittent signal: Deviation from $u_n(t) \alpha t^{\gamma n}$ at small t Useful measures of intermittency:

Flatness: $\kappa(t) = u_4(t) / (u_2(t)^2)$

Temporal Intermittency in the Aggregate Phase ime dependence of Flatness

 $\kappa(t)=u_4(t)\,/\,(u_2(t)^2)\,$ with $\,u_n(t)=<$ (M(t) – M(0) $)^n>$



Analytic results: Pure aggregation limit

- Moments $u_n(t) = \langle (M(t) M(0)) \rangle$
- Define generalized autocorrelation function

$$H_{i,j}(t) = \langle M_{i,j}(t) | M_{0,L}(0) \rangle - \langle M_{i,j}(t) \rangle \langle M_{0,L}(0) \rangle$$

where $M_{i,j}$ is the mass between sites i and j

Write time evolution equation for H_{i,j}(t)

Take continuum limit to convert recursions to PDE for H(x,y,t) Can be solved by 'folding' triangle to square Result:

 $u_2(t) \sim A_0 t \log (A_1 Dt/L^2)$ A₀, A₁ are constants, Dt << L²

 $u_{2n}(t) \sim -L^{2n-2} t g_{2n} \log (Dt/L^2)$

	<mark>Condensate</mark> Phase (w < w _c)	$\frac{\text{Normal Phase}}{(w > w_c)}$	$\frac{\text{Critical Point}}{(w = w_c)}$
Statics	$P(M) \rightarrow$ Condensate tail Giant Fluctuations: $\Delta M \propto L$	$P(M) \rightarrow$ Gaussian tail Normal Fluctuations: Δ <i>M</i> ∝ √ <i>L</i>	$P(M) \rightarrow$ Non-Gaussian tail Large Fluctuations: Δ $M \propto L^{2/3}$
Dynamics	$M(t) \rightarrow Strongly$ intermittent Flatness diverges as $t / L^2 \rightarrow 0$	M(t) → Not intermittent No divergence of Flatness.	<i>M(t)</i> → Intermittent Flatness diverges at small <i>t</i> .

Reflecting: No Exit at Left



Directed Stack Hopping



Conclusion

Condensation phase transition in open system, with no mass conservation

Key signature: Fluctuations

- Giant number fluctuations in the condensate
- Total mass shows temporal intermittency

Related phase transitions

- With reflecting boundary conditions
- With directed motion of masses

Open question

Do other systems which show clustering and giant fluctuations also exhibit temporal intermittency?

Analysed by Monte Carlo simulations and by solving for P(m) assuming factorizability: $P(m_1,m_2) = P(m_1)P(m_2)$

$$\frac{\partial P_m}{\partial t} = -(D+w)[1+s]P_m + wP_{m+1} + wsP_{m-1} + D\sum_{n=1}^m P_n P_{m-n}$$

where $s = 1 - P_0$ is the probability that the site is occupied

Find: Phase transition as the density is increased



- In the normal phase, $P_m \sim e^{-m/m_0}$
- At the critical point, $P_m \sim m^{-\tau}$; $\tau = 5/2$
- Beyond the critical point, $P_m \sim m^{-\tau} + Condensate$ A single site holds a finite fraction of particles ----Bose condensation, but in real space

[S. N. Majumdar, S. Krishnamurthy, M. Barma, J Stat Phys (2000)]

Analysed by Monte Carlo simulations and by solving for P(m) assuming factorizability: $P(m_1, m_2) = P(m_1) P(m_2)$

Find: In Aggregate phase, a single site holds a finite fraction of ---- akin to Bose condensation, but in real space



R. Rajesh and S. Majumdar; **R.** Rajesh and S. Krishnamurthy

Phase boundary found through factorizability is exact [Phys Rev E (2001)] Given the rules of molecular trafficking, can one model some aspects of processes within the cell?

(e.g. motion and processing of biomolecules in the Golgi)



(Molecular Biology of the Cell, B Alberts, A Johnson, J Lewis, New York: Garland ; 2002.)

