

## 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 charact from the closed case.



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

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

# •P(m) : Long 'Condensate tail' ... P(M) $\approx$ A exp(-M/M<sub>0</sub>) at

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  $t / \tau \rightarrow 0$ [ $\tau$  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<sub>i,j</sub>(t)

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

 $u_2(t) \sim A_0 t \log (A_1 Dt/L^2)$  A<sub>0</sub>, A<sub>1</sub> are constants, Dt << L<sup>2</sup>

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

	<mark>Condensate</mark> Phase (w < w <sub>c</sub> )	Normal Phase (w > w <sub>c</sub> )	$\frac{\text{Critical Point}}{(w = w_c)}$
Statics	$P(M) \rightarrow$ Condensate tail Giant Fluctuations: $\Delta M \propto L$	$P(M) \rightarrow$ Gaussian tail Normal Fluctuations: $\Delta M \propto \sqrt{L}$	$P(M) \rightarrow$ Non-Gaussian tail Large Fluctuations: $\Delta M \propto L^{2/3}$
Dynamics	$M(t) \rightarrow Strongly$ intermittent Flatness diverges as $t / L^2 \rightarrow 0$	<i>M(t)</i> → 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. )

