Percolation of a collection of finite random walks

a model for gas permeation through thin polymeric membranes

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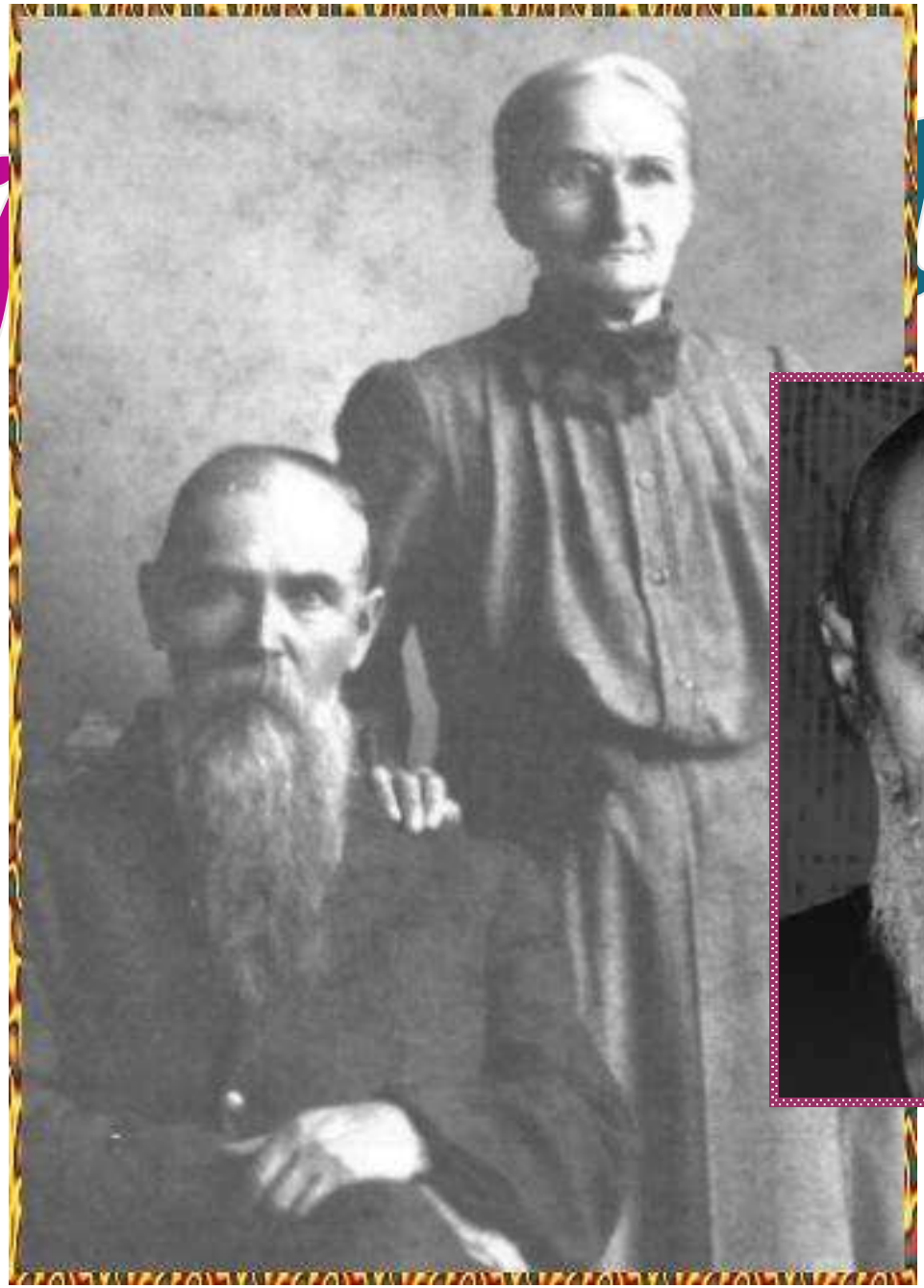
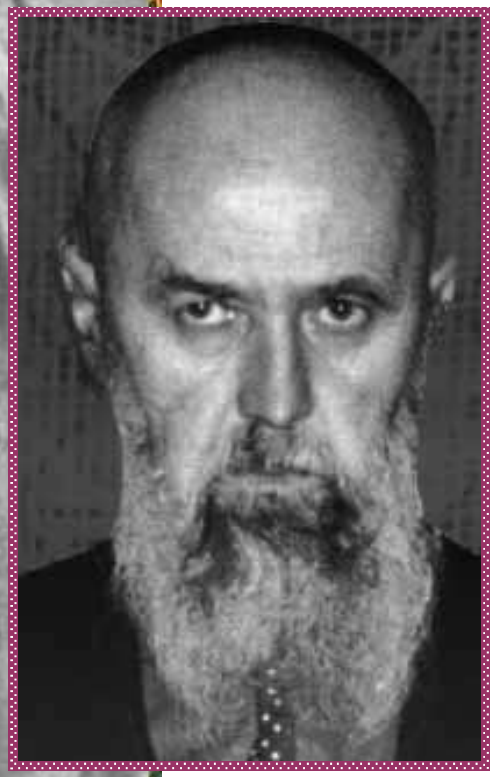
J. Phys. **A37**, L337 (2004); cond-mat/0404266
J. Phys. **C17,** S1817 (2005); cond-mat/0501302
JSTAT . P04002 (2007); cond-mat/0703039
…

Supported by:
NSF-DMR: Materials Theory

Happy Birthday





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A Symposium of

Mathematical Chemistry

Mathematician

sharp mind

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Theoretical Physicist

fuzzy logic

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fuzzy logic

pencil & paper

computer

Chemist

courageous heart

Lattices and Trajectories

Percolation of *correlated* bonds on a square lattice

- Motivation
- The Model and the Problem
- Results: Simulation & Analytic
- Outlook

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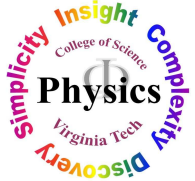


Permeation of gas molecules

through thin polymeric membranes

- Saran-wrapped garlic in a fridge!
- Experiments by C.M. Laot and E. Marand
- Effects on gas transport due to
  - cooling rate in membrane preparation
  - physical aging
  - orientation (stretching)

http://scholar.lib.vt.edu/theses/available/etd-12012001-133140/

Percolation Problem in 2-D

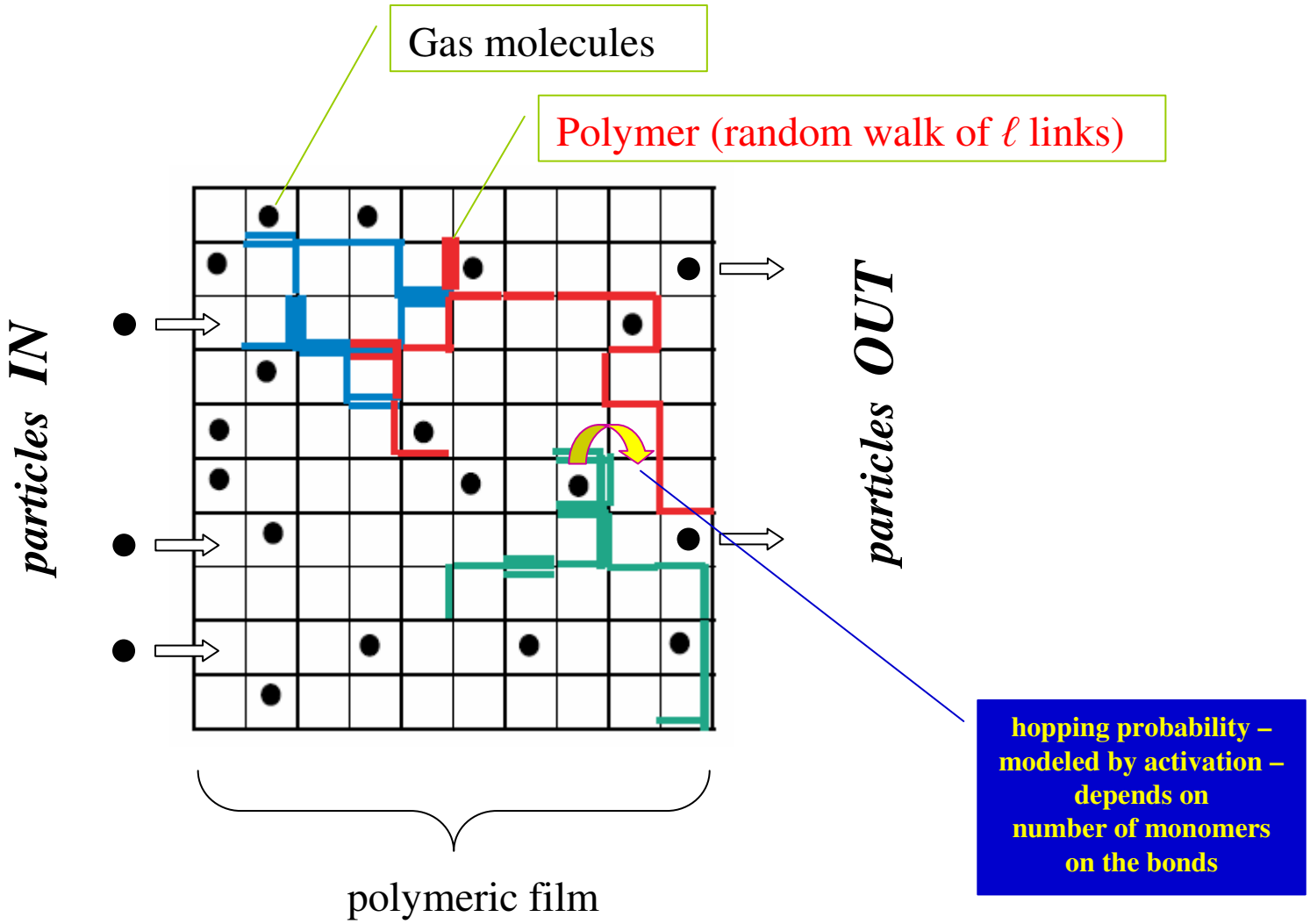
- Percolation on square lattice (site and bond) well known
- What happens if the bonds (in this case) are correlated?

Model for gas transport

Start with just 2-D

Trajectories on a square Lattice

Model for gas transport



MODEL + PROBLEM

Percolation Problem in 2-D

- Percolation on square lattice (site and bond) well known
- What happens if the bonds (in this case) are correlated?
- Simplified (and dual) problem:
  - For $T = 0$, particles cannot cross occupied bonds
  - If occupied bonds (from the ℓ-mers) span system, there'd be no particle current!
  - …percolation of *correlated* bonds

Percolation Problem in 2-D

- $p \equiv$ density of occupied bonds; $p_c = 1/2$ on square lattice
- $\rho \equiv$ density of (randomly placed) *monomers* (= *mass* density)
- $\rho \neq p$ due to multiple occupancies: $1 - p = (1 - A^{-1})^{\rho A} \rightarrow exp(-\rho)$
- What happens if monomers are joined to form ℓ-*mers*?
- What happens to p-ρ relationship?

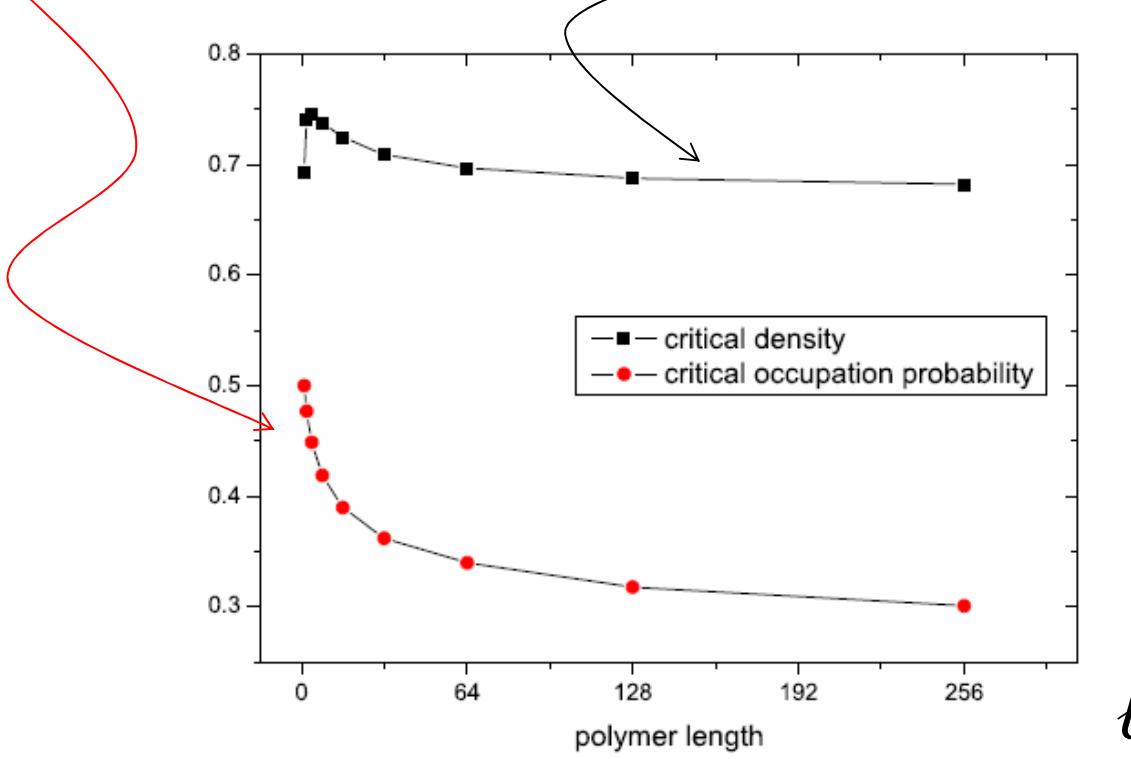
  …if ℓ-*mers* are just simple random walks
- Occupied bonds are *correlated*: What's $p_c(\ell)$ or $\rho_c(\ell)$?

Results: Analytic & Simulation

- ü p-ρ relationship (even for finite systems)
- ü Probability of spanning for single RW
  - *all* monomers linked into a single polymer
  - of course, *no* singularities here: Prob is a smooth function of ρ.
- ü Probability of *multiple* occupation
  - useful for gas transport model for finite T
  - based on results of Antal, Hilhorst and Zia, *J. Phys*. **A35**, L337 (2002)
    …for *multiple* occupation of bonds by a single RW.

Results: Analytic & Simulation

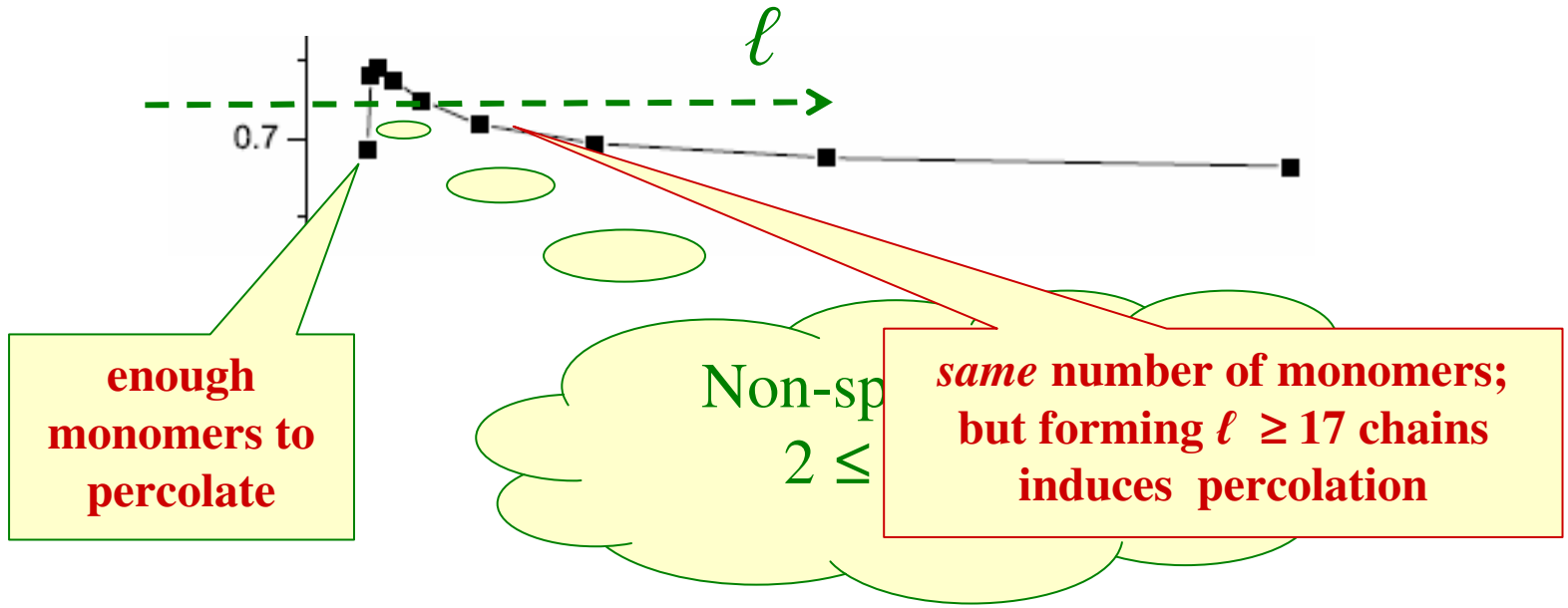
- $p_c(\ell)$ and $\rho_c(\ell)$



RESULTS

Results: Analytic & Simulation

- $p_c(\ell)$ and $\rho_c(\ell)$
- "re-entrant" behavior with increasing ℓ (fixed ρ)



Results: Analytic & Simulation

- $p_c(\ell)$ and $\rho_c(\ell)$
- "re-entrant" behavior with increasing ℓ

  …"*postdiction*" – words w/o understanding

Results: Analytic & Simulation

- $p_c(\ell)$ and $\rho_c(\ell)$
- "re-entrant" behavior with increasing ℓ

  …"*postdiction*" – words w/o understanding
- critical behavior in $\ell = 1$ (usual) universality class
- ⋮

Outlook

- Relationship between this problem and percolation of random ellipses?
- Fancier RW's: anisotropic (effects of "orientation"), non-Gaussian (e.g., self-avoiding), etc.
- Effects of finite T : diffusion, steady current, etc.
- Generalizations to 3-D: (both math and physics puzzles)
- The *real* problems:
  - What happens when polymer dynamics (aging phenomena) is added?
  - How to introduce different cooling rates?
  - ⋮

sharp minds + courageous hearts
sorely needed!!

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