Many random walkers: rare events and long-range correlations

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Overview

1. Random walks and diffusive rare events
2. Results on first-passage times
3. Energetic random walkers
4. Long-range correlations

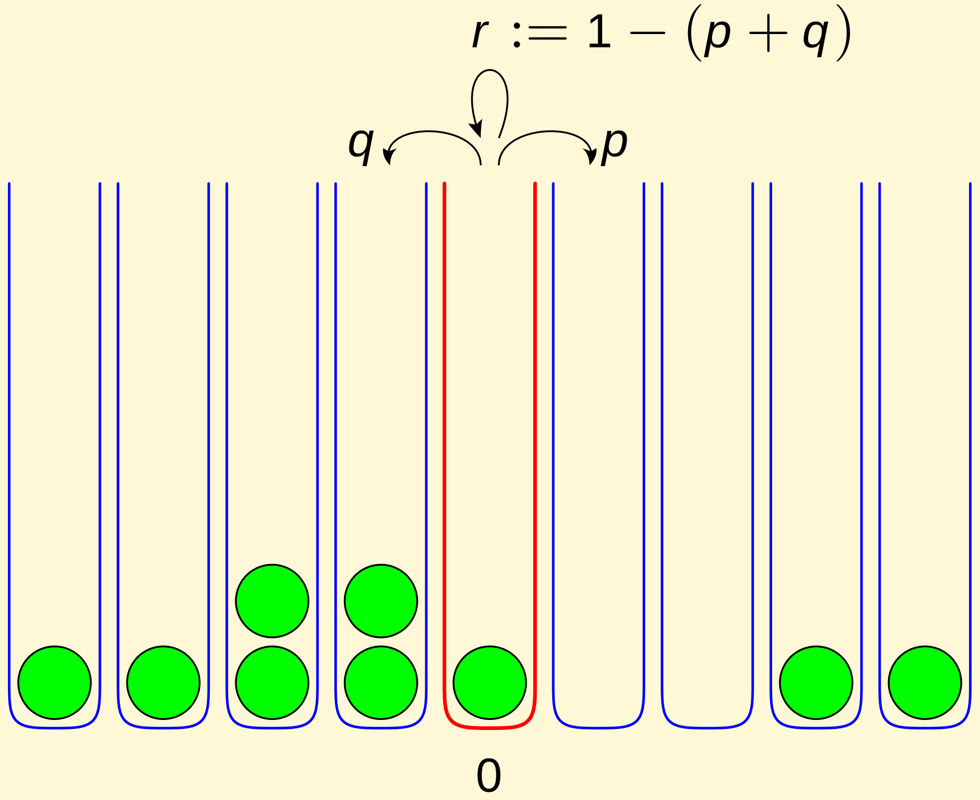
Random walks
and diffusive rare events

Diffusive rare events

- Diffusive rare event: accumulation of diffusing particles
- No activation energy
- Glassy behaviour
  - hard disc fluid
  - Ritort backgammon model
- Blockage of membrane pores (Weiss & Argyrakis, 2006)
- General question:

How long until large density fluctuation occurs?

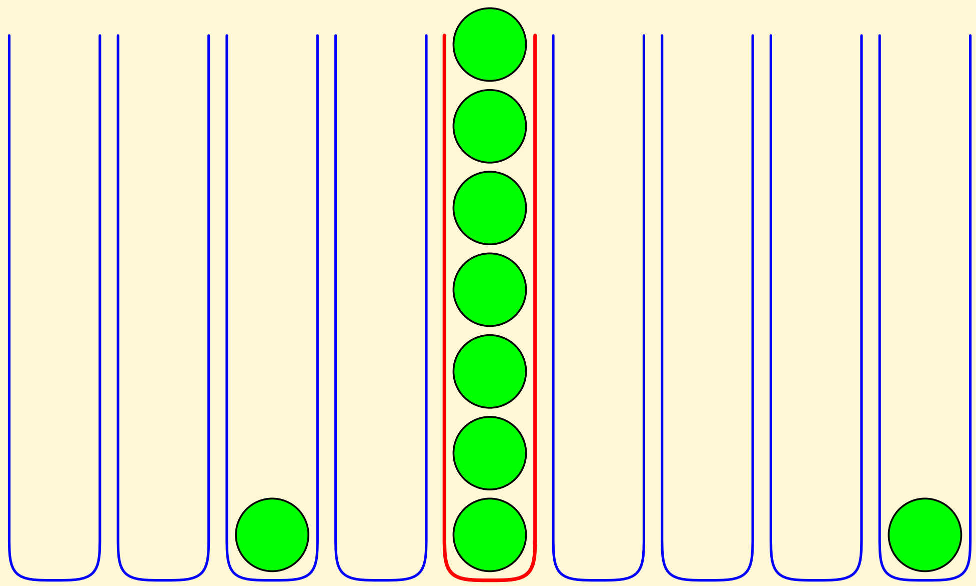
- N independent random walkers; discrete time



- Configurations: $\mathbf{s} = (s_1, \ldots, s_N) \in \{1, \ldots, V\}^N$
- Density $\rho := N/V$

- Event with k walkers at distinguished site 0:

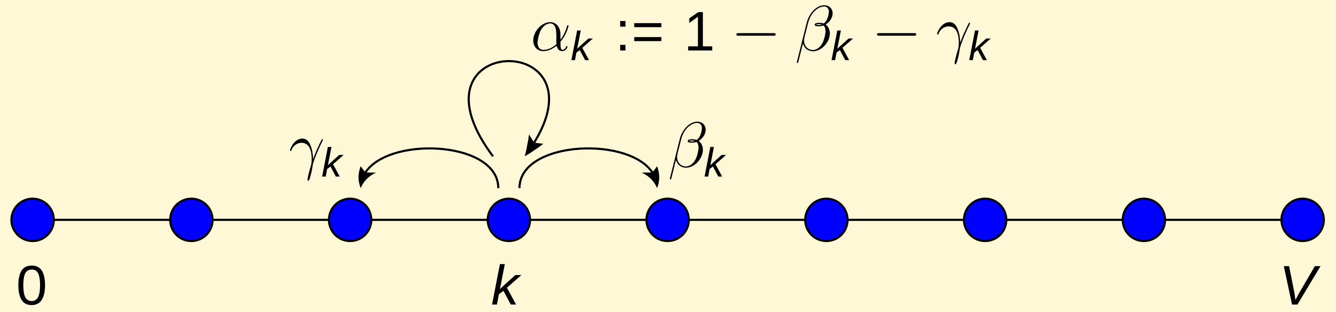
$$S_k := \{\mathbf{s} : \sum_i \delta(s_i, 0) = k\} = \{k \text{ walkers at site } 0\}$$



- When first arrive at S_k?   mean first-passage time τ_k^{FP}
- Random initial conditions outside S_k

First-passage times: results

- Walkers jump to any site: Ehrenfest urn model
- Dynamics of n_0 is Markov chain:



$$\gamma_k = \frac{k}{N}; \qquad \beta_k = \frac{N-k}{N}\frac{1}{V-1}$$

- Conditioning gives recurrence relation:

$$\tau_k^+ = \alpha_k(1 + \tau_k^+) + \beta_k(1 + \tau_{k+1\to k+1}) + \gamma_k(1 + \tau_{k-1\to k+1})$$

$$\tau_k^+ = \frac{1}{\beta_k} + \frac{\gamma_k}{\beta_k}\tau_{k-1}^+$$

First-passage and recurrence

- Recurrence time τ_A^{rec} = time from $A \longrightarrow A$

- From S_k almost certainly drop to S_{k-1}
- Reach "random" condition, then first-passage process:

$$\tau_k^{\text{rec}} \simeq [1 \times \mathbb{P}(\text{stay})] + [\tau_k^{\text{FP}} \times \mathbb{P}(\text{leave})]$$
$$\simeq 1 + \gamma_k(\tau_k^{\text{FP}} - 1)$$

- Exact relation for mean-field:

$$\tau_k^{\text{rec}} = 1 + \beta_k \tau_{k+1}^{-} + \gamma_k \tau_{k-1}^{+}$$

- Approx:

$$\tau_k^{\text{FP}} \simeq \frac{\tau_k^{\text{rec}}}{\gamma_k}$$

Asymptotics

- Kac recurrence theorem:

$$\tau_A^{\text{rec}} = \frac{1}{\mathbb{P}(A)}$$

- Apply to S_k:

$$\tau_k^{\text{rec}} = \frac{1}{|S_k| \,/\, |\Omega|} = \frac{V^N}{\binom{N}{k}(V-1)^{N-k}}$$

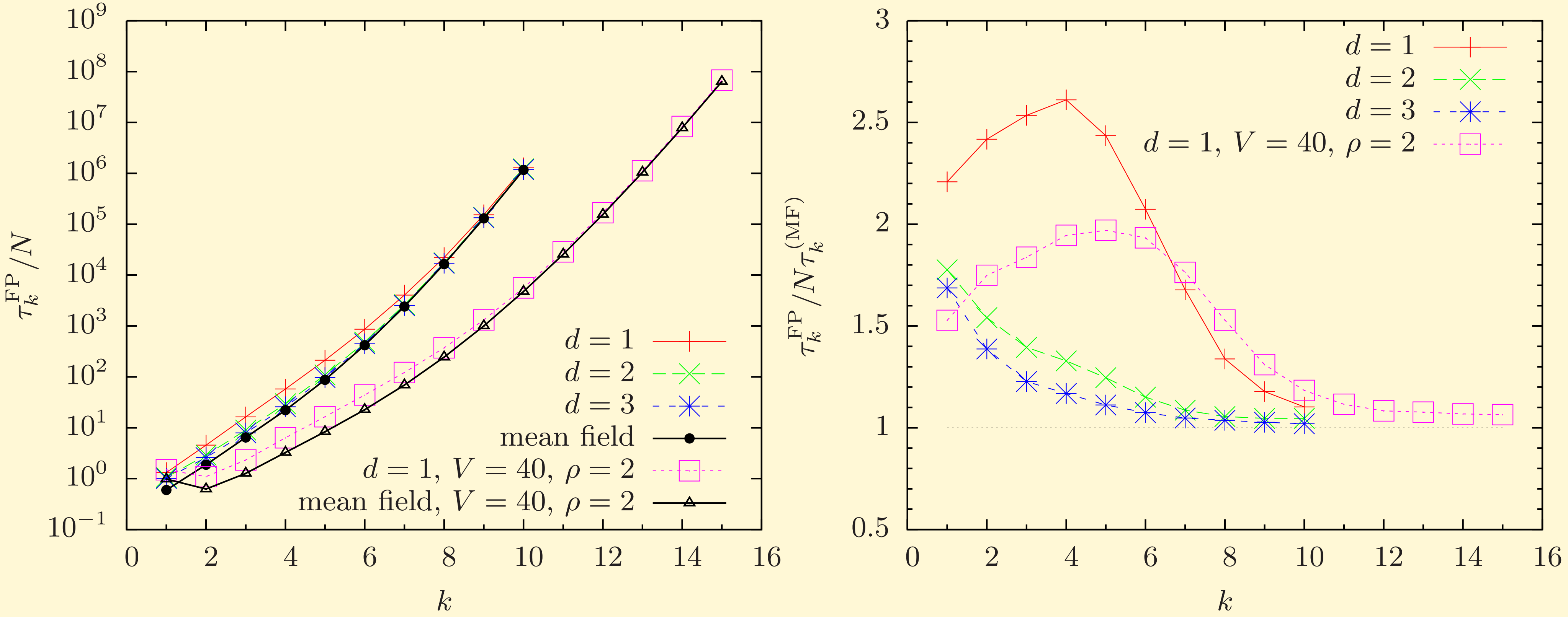
- Asymptotics: large N, V; fixed $\rho = N/V$; fixed $\rho \ll k \ll N$

$$\tau_k^{\text{rec}} \sim k!\, \rho^{-k} \exp(\rho)$$

- First-passage asymptotics:

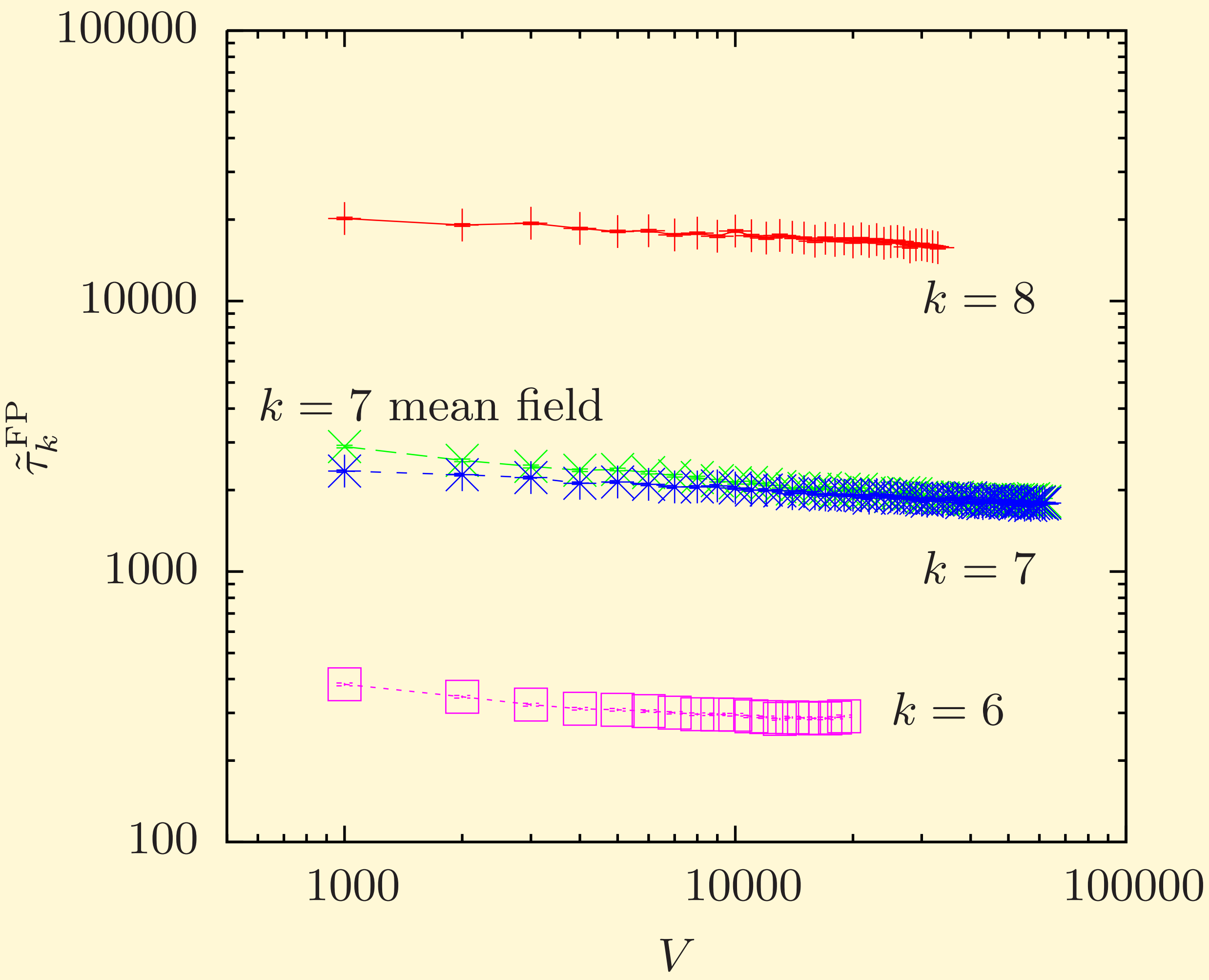
$$\frac{1}{N}\tau_k^{\text{FP}} \simeq (k-1)!\, \rho^{-k} \exp(\rho)$$

Numerics and mean-field



Rare events anywhere in system

- What if fluctuation can occur anywhere in system?
- Set $\tilde{S}_k$ roughly V times larger



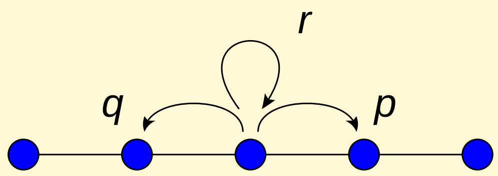
Summary

- Asymptotic first-passage time to density fluctuations
- Mean-field and spatial cases similar
- Fluctuations anywhere in system

- Open questions
  - Good algorithm for diffusive rare events
  - Exact results for fluctuations anywhere in system

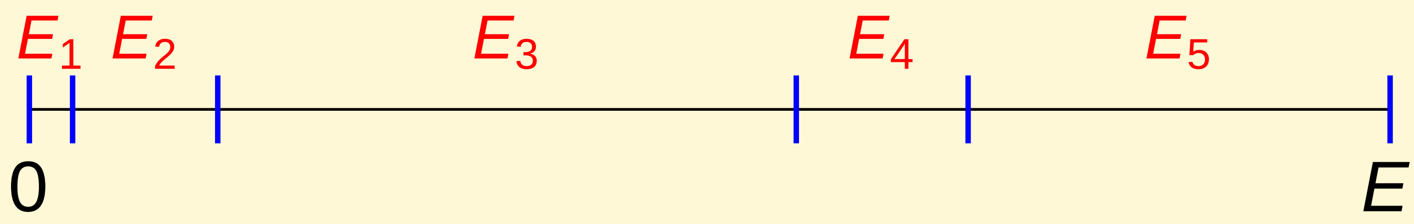
Energetic random walks

Random walkers with energy



- Particles: random walks
- Carry continuous "energy"; motion unaffected by energy
- Related to random-halves model (Eckmann, Young, Lin)

- Energy E redistributed microcanonically among n particles:
- Insert $n-1$ partitions randomly



- Particle energy distribution:

$$\mathbb{P}(E_1 > e) = \left(\frac{E-e}{E} \right)^{n-1}$$

Reservoirs

- Reservoirs with densities ρ_0, ρ_{L+1}; temperatures T_0, T_{L+1}
- Number of particles visible in reservoir with density ρ:

$$\mathbb{P}(n) = \exp(-\rho)\frac{\rho^n}{n!}$$

- Energy of particles from reservoir at temperature T:

$$\mathbb{P}(E) = \frac{1}{T}e^{-E/T}$$

Equilibrium

- Equilibrium conditions: $\rho_0 = \rho_{L+1}; \quad T_0 = T_{L+1}$
- In equilibrium, whole joint distribution factorises:

$$P(\mathbf{E}; \mathbf{n}) = \prod_{i=1}^{L} P(n_i) P(E_i | n_i)$$

- Energy distribution: sum of independent random variables:

$$P(E|n) = \frac{\beta^n E^{n-1} e^{-\beta E}}{\Gamma(n)}$$

Density and energy profiles

- Density profile: $\rho_i := \langle n_i \rangle$

$$\rho_i^{t+1} = p\,\rho_{i-1}^t + r\,\rho_i^t + q\,\rho_{i+1}^t$$

- Energy profile:

$$\langle E_i \rangle_{t+1} = p\,\langle E_{i-1} \rangle_t + r\,\langle E_i \rangle_t + q\,\langle E_{i+1} \rangle_t$$

- Non-equilibrium steady state: $\langle E_i \rangle =: \rho_i T_i$

$$p\,\rho_{i-1} T_{i-1} + r\,\rho_i T_i + q\,\rho_{i+1} T_{i+1} = \rho_i T_i$$

- Non-equilibrium joint distribution $P(\mathbf{E}; \mathbf{n})$ does not factorise

Long-range energy correlations

Previous work

- Fluctuating hydrodynamics, experiments (Dorfman, Kirkpatrick, Sengers $\sim$ 1980)
- Mode-coupling theory
- Oscillator chain (Kipnis et al., 1982)
- Stochastic lattice gas (Spohn, 1983)
- Lattice-gas cellular automaton (Boon et al., 1996)
- Random-halves model (Lin & Young, 2007)

Spatial correlations of energy

- Spatial correlations

$$C_{i,j} := \langle E_i E_j \rangle - \langle E_i \rangle \langle E_j \rangle$$

- Notation:

$$(\Delta_1 C)_{i,j} := pC_{i-1,j} + rC_{i,j} + qC_{i+1,j}$$

- Find in steady state

$$\langle E_i \rangle = \Delta_1 \langle E_i \rangle$$
$$\langle E_i \rangle \langle E_j \rangle = \Delta_1 \Delta_2 \left[\langle E_i \rangle \langle E_j \rangle \right]$$

- From site i, energy s_i^+, s_i^- and l_i^+, l_i^- particles move right, left

$$\langle E_i E_j \rangle = \Big\langle \left[E_i + (s_{i-1}^+ + s_{i+1}^-) - (s_i^+ + s_i^-) \right] \times \left[E_j + (s_{j-1}^+ + s_{j+1}^-) - (s_j^+ + s_j^-) \right] \Big\rangle$$

Spatial correlations II

- Evaluate products:

$$\left\langle s^+_{i-1} s^+_{j+1} \right\rangle = \left\langle s^+_{i-1} \right\rangle \left\langle s^+_{j+1} \right\rangle \quad \text{provided} \quad i - 1 \neq j + 1$$

$$\left\langle s^+_i \middle| E_i, l^+_i, n_i \right\rangle = \frac{l^+_i}{m_i} E_i; \qquad \left\langle s^{+2}_i \middle| E_i, l^+_i, n_i \right\rangle = \frac{l^+_i (l^+_i + 1) E^2_i}{n_i (n_i + 1)}$$

- Finally obtain:

$$C_{i,j} = \Delta_1 \Delta_2 C_{i,j} + 2\nu_{ij}$$

- Define long-range part

$$g_{i,j} := C_{i,j} - 2\kappa_i \delta_{ij}$$

- Then

$$g_{i,j} = \Delta_1 \Delta_2 g_{i,j} + 2\mu_i \delta_{ij}$$

- Source of long-range correlations:

$$\mu_i := p\kappa_{i-1} + q\kappa_{i+1} + (r-1)\kappa_i$$

with

$$\kappa_i := \left\langle \frac{E_i^2}{n_i + 1} \right\rangle$$

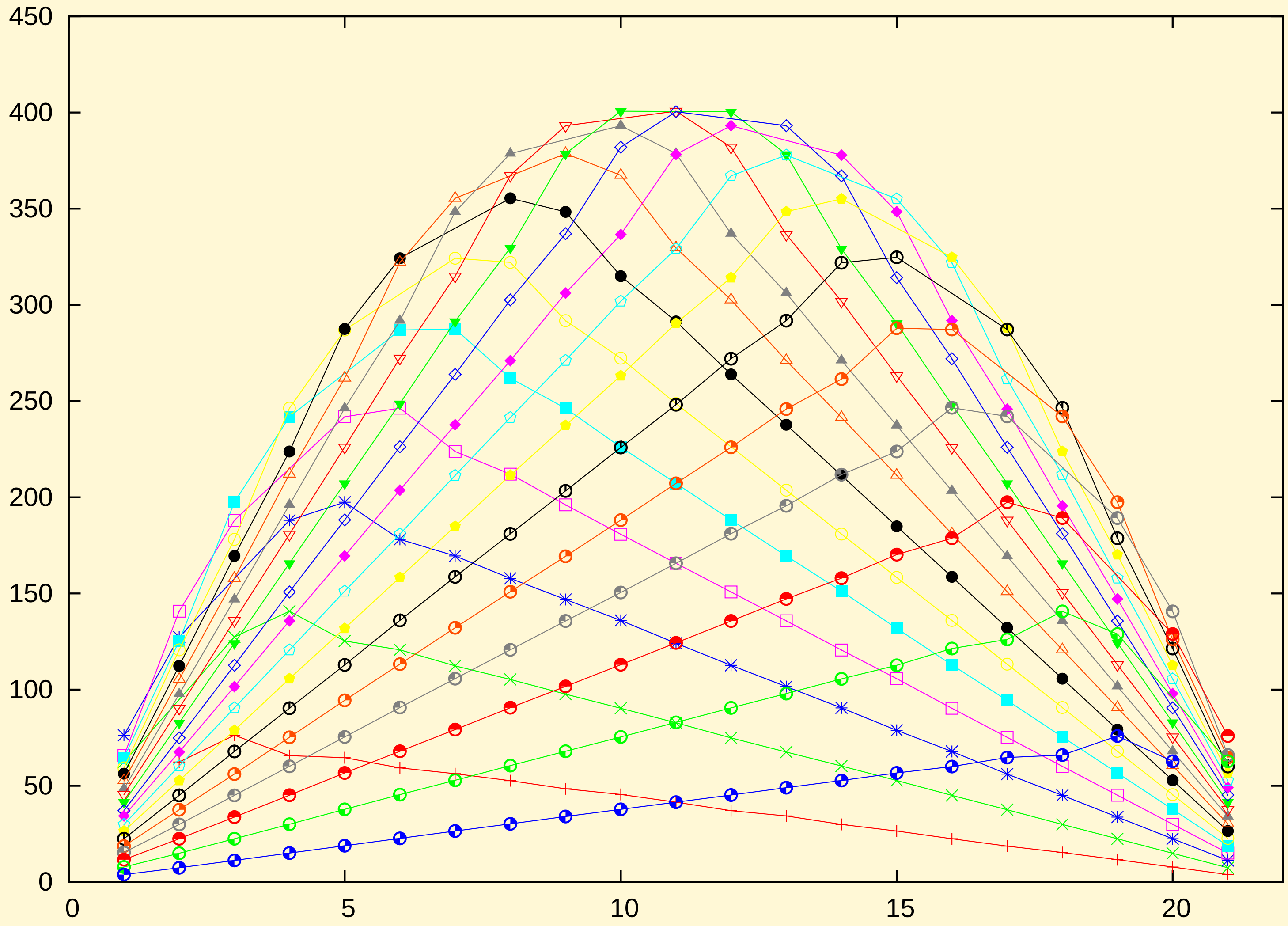
- Assume local equilibrium for marginal distribution at site i (Ravishankar & Young, 2007)

$$\kappa_i = \rho_i T_i^2 = \frac{\rho_i}{\beta_i^2}$$

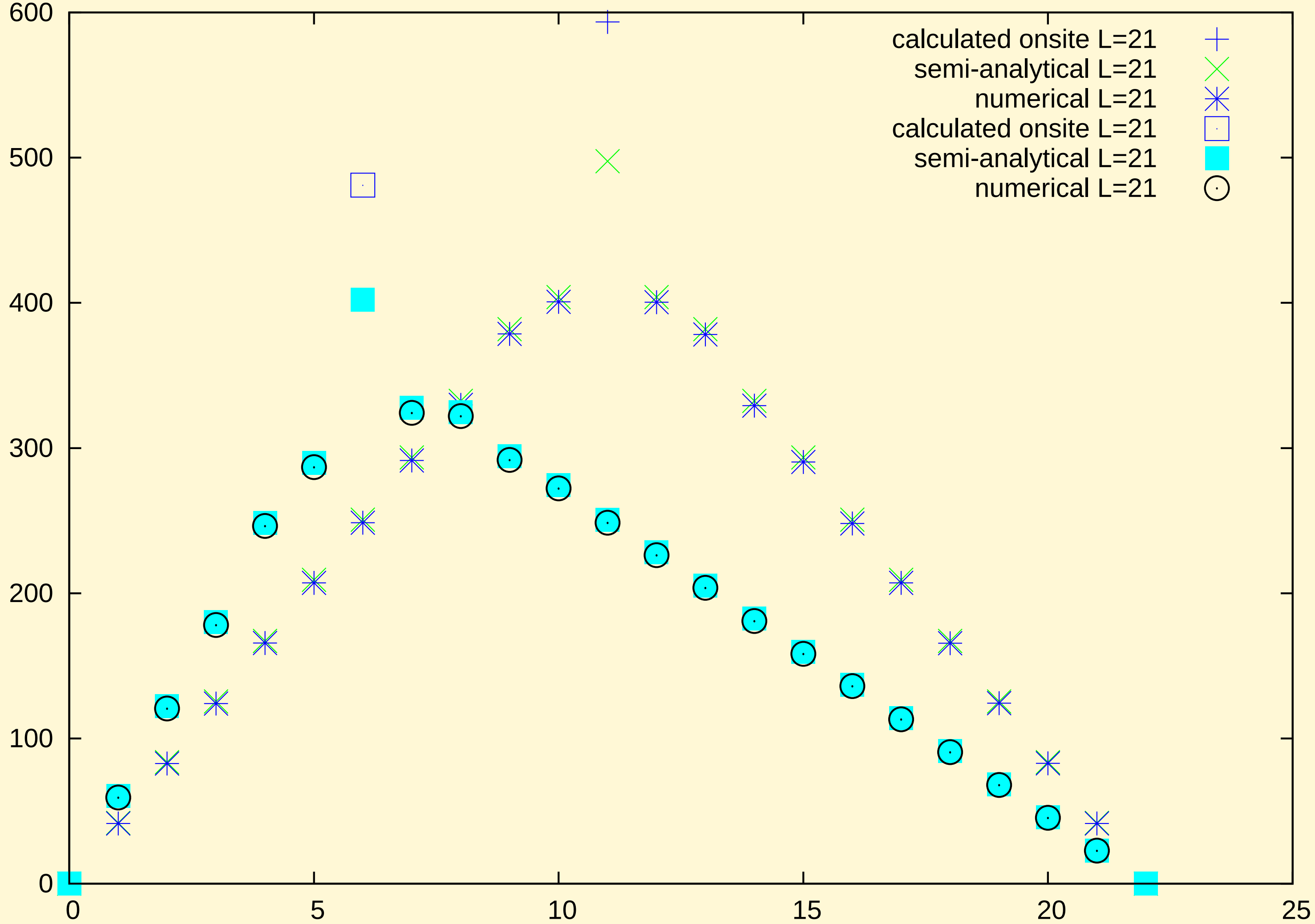
- Source μ_i assuming local equilibrium:

$$\mu_i \simeq 2D\rho(x)[\nabla T(x)]^2$$

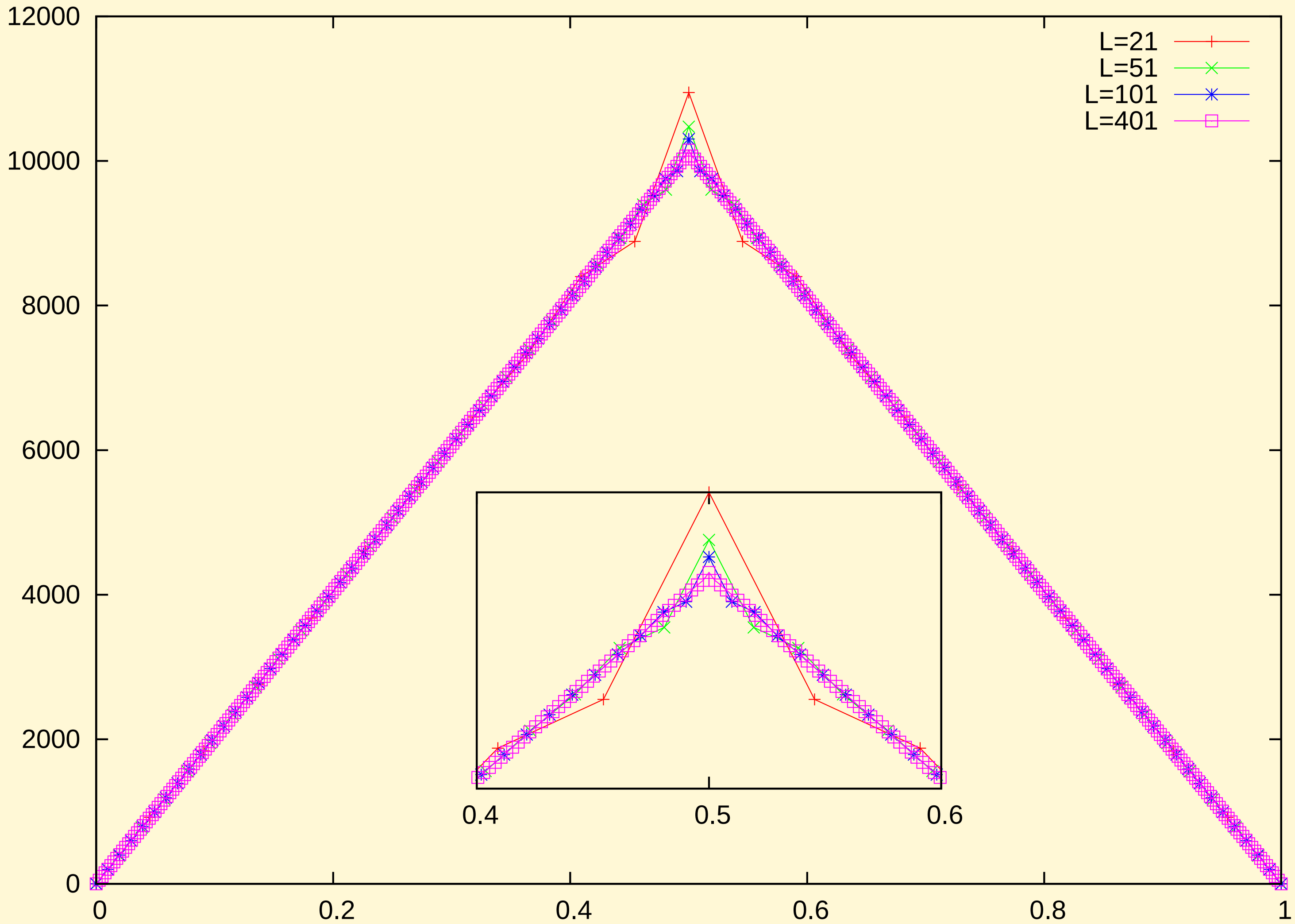
Numerical: $L = 21$, no density gradient



Comparison of numerics with analytical



Scaling with system size (semi-analytical)



Summary

- Exact equation for spatial energy correlations
- Local equilibrium assumption agrees with numerics

- Open questions:
  - Exact solution of correlation equation
  - Case where dynamics depends on energy

- Money:
  - PROFIP programme
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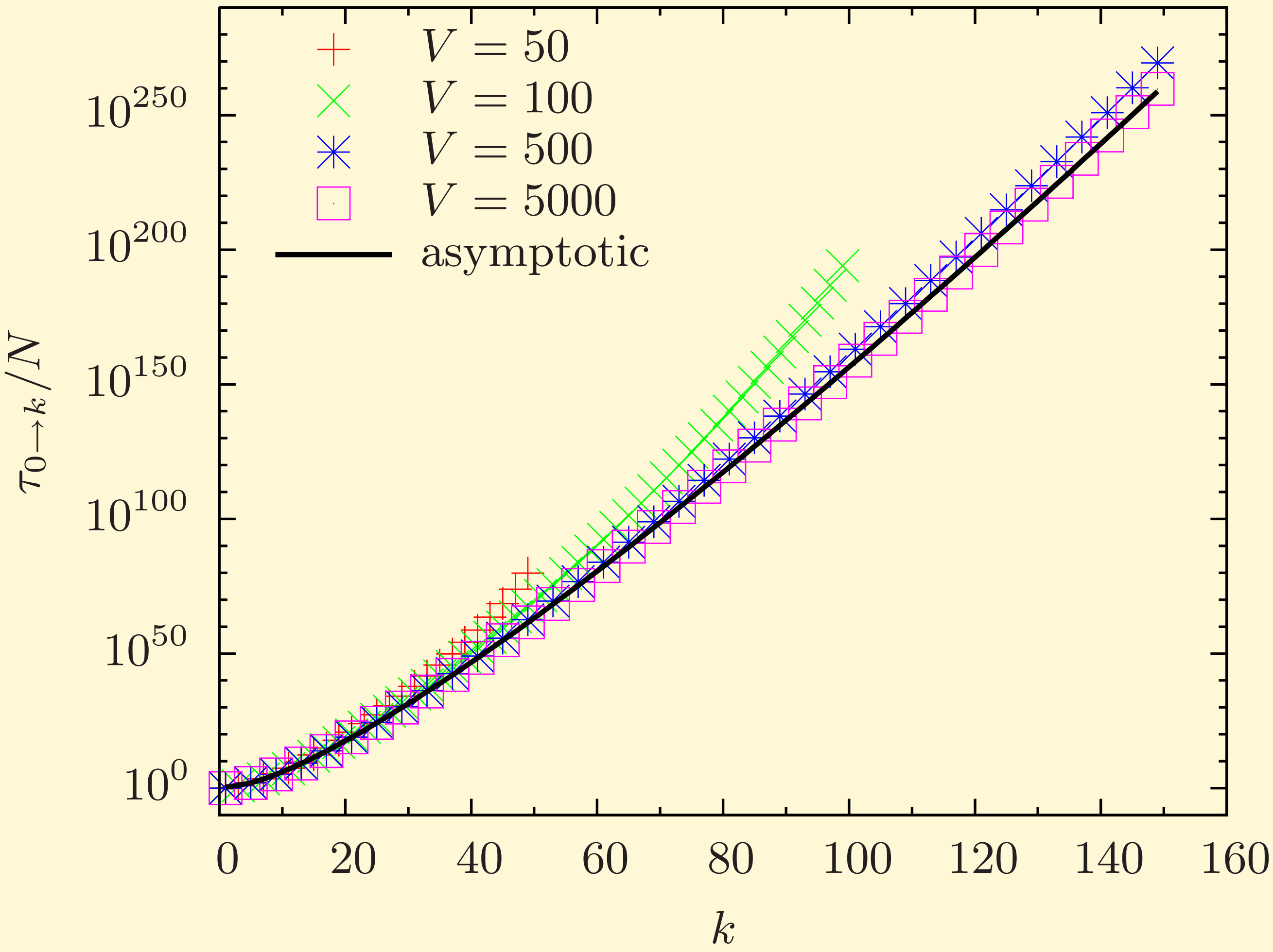
Appendix

Exact mean-field and asymptotics



Master equation

$$P_{t+1}(n_1, E_1; n_2, E_2; \ldots ; n_L, E_L) =$$

$$\sum_{\{m_i\}} \sum_{\{l_i^\pm\}} \int_{\{e_i\}} \mathrm{d}\, e_i \int_{\{s_i^\pm\}} \mathrm{d}\, s_i^\pm \, P_t(m_1, e_1; m_2, e_2; \ldots ; m_L, e_L)$$

$$\times \prod_i \delta \left(n_i - [m_i + (l_{i-1}^+ + l_{i+1}^-) - (l_i^+ + l_i^-)] \right)$$

$$\times \prod_i \delta \left(E_i - [e_i + (s_{i-1}^+ + s_{i+1}^-) - (s_i^+ + s_i^-)] \right)$$

$$\times \prod_i \mathbb{P} \left(s_i^+, s_i^- \,\middle|\, l_i^+, l_i^-, m_i, e_i \right) \times \prod_i \mathbb{P} \left(l_i^+, l_i^- \,\middle|\, m_i \right)$$

$$\mathbb{P} \left(l_i^+, l_i^- \,\middle|\, m_i \right) := \binom{m_i}{l_i^+} \binom{m_i - l_i^+}{l_i^-} p^{l_i^+} q^{l_i^-} r^{m_i - l_i^+ - l_i^-}$$

$$\mathbb{P} \left(s_i^+, s_i^- \,\middle|\, l_i^+, l_i^-, m_i, e_i \right) :=$$

$$\frac{\Gamma(m_i)}{\Gamma(l_i^+)\Gamma(l_i^-)\Gamma(m_i - l_i^+ - l_i^-)} (s_i^+)^{l_i^+ - 1} (s_i^-)^{l_i^- - 1} \frac{(e_i - s_i^+ - s_i^-)^{m_i - l_i^+ - l_i^- - 1}}{e_i^{m_i - 1}}$$