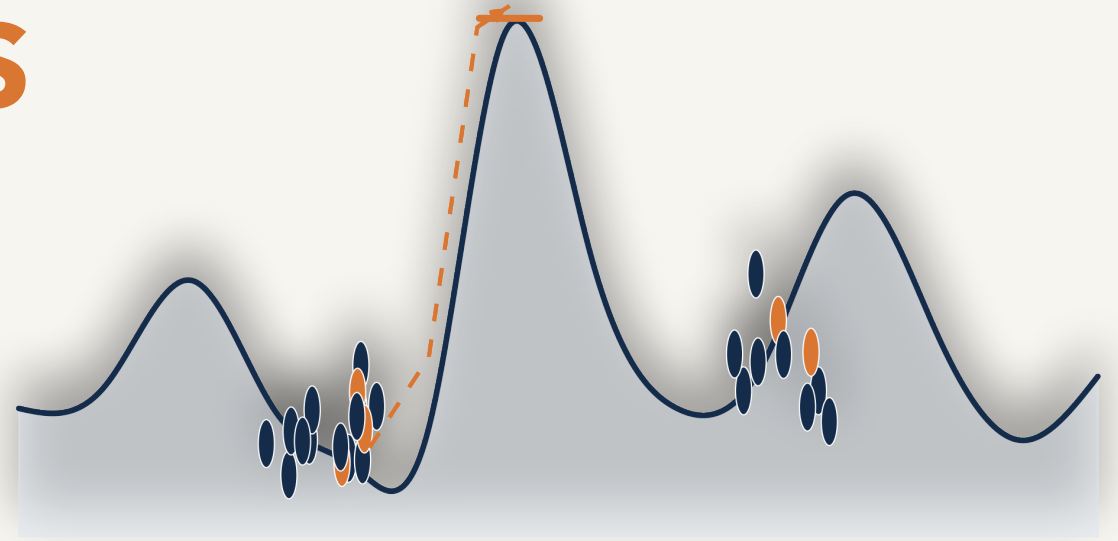


ACTIVATION BEYOND **ARRHENIUS**

Interactions & Escape Dynamics



The Institute of Mathematical Sciences, Chennai
ICTS MFT Conference [2026]

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OHAD SHPIELBERG



Physical Review E 109 (3), L032101 [2024]

The Journal of Chemical Physics 160 (13) [2025]

The Journal of Chemical Physics 163 (22) [2025]

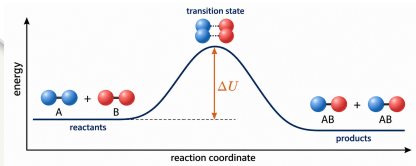


ACTIVATION IS EVERYWHERE

Very different phenomena share the same rare-event logic

CHEMICAL REACTIONS

molecules cross an activation barrier



Potential
Energy

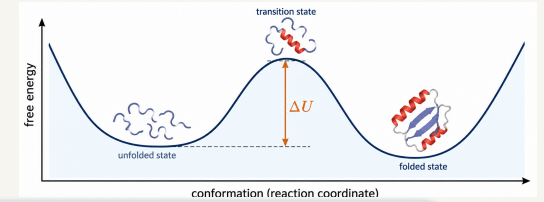
rare event

ΔU

reaction coordinate

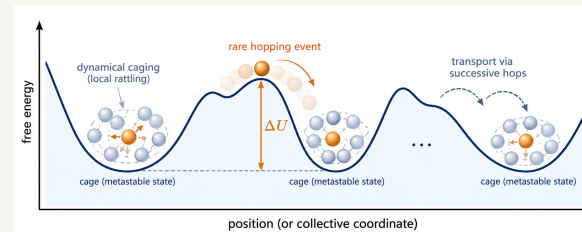
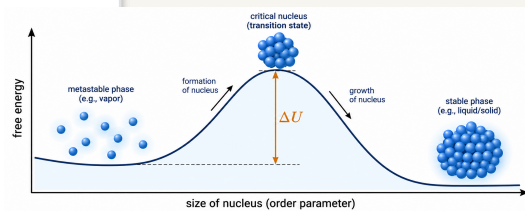
PROTEIN FOLDING

rare transitions between metastable states



NUCLEATION

a critical fluctuation creates a new phase



DYNAMIC CAGING & TRANSPORT

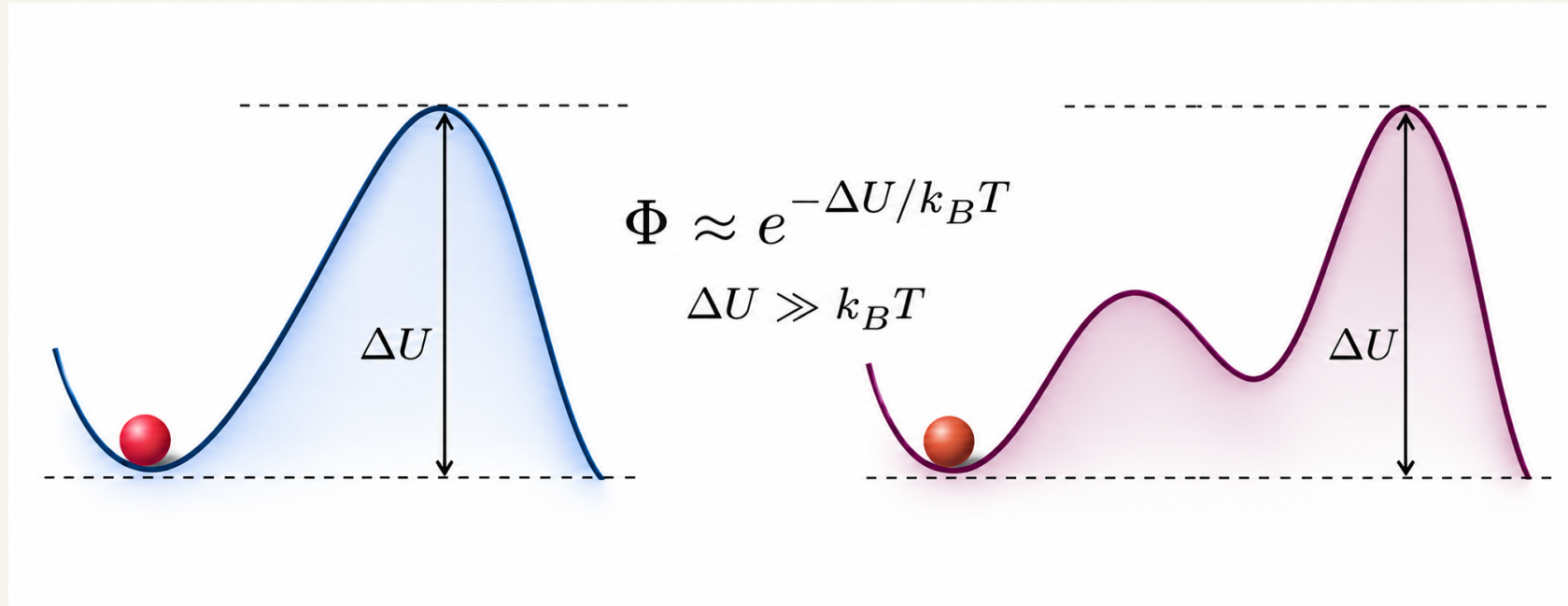
escape from a dynamical confinement created by other particles

Different systems. Same question: how does escape happen?

A CENTURY OF UNIVERSALITY [Kramers 1940]

Very different landscapes can share the same activation barrier

Hanggi et al, Reviews of modern physics, 62(2):251, 1990



Activation barrier: Escape is an **activated process**, controlled by the energy barrier

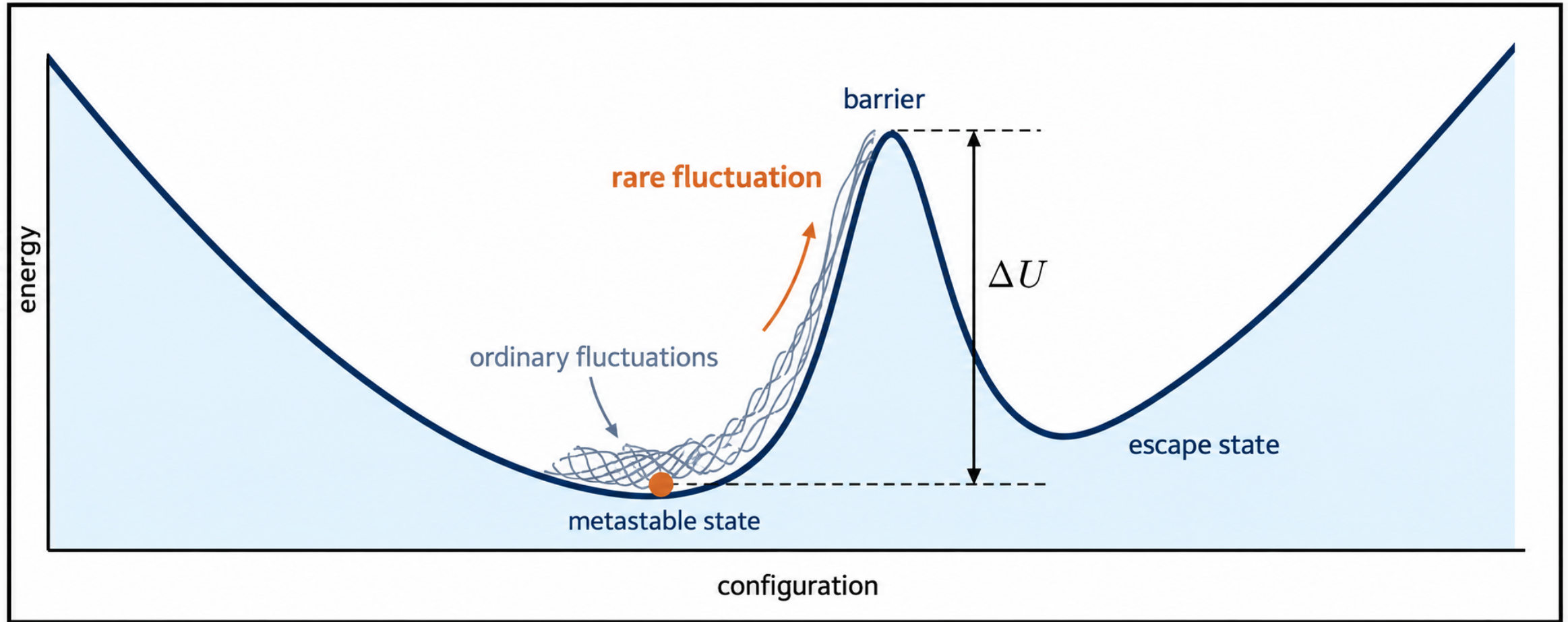
Universal exponential scaling: The leading Arrhenius dependence is **independent of the detailed shape** of the potential $U(x)$, only the activation barrier matters

Potential shape → prefactor: The detailed landscape affects the **sub-exponential prefactor**

ONLY THE BARRIER MATTERS

Escape is a rare fluctuation that reaches the barrier

Kamenev, Field Theory of Non-Equilibrium Systems
Langer, Annals of Physics 54, 258-275 (1969)



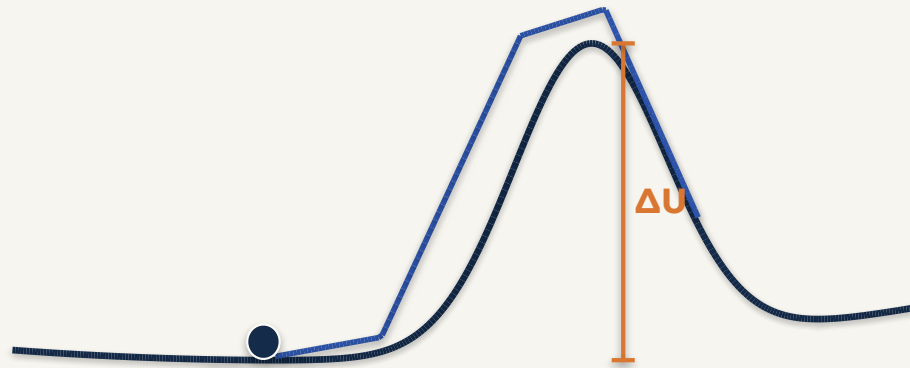
Only rare trajectories reach the barrier

INSTANTONS/LEAST ACTION yield EXPONENTIAL

WHAT CHANGES IN A MANY-BODY SYSTEM?

Activation is still required – but the activated object becomes collective

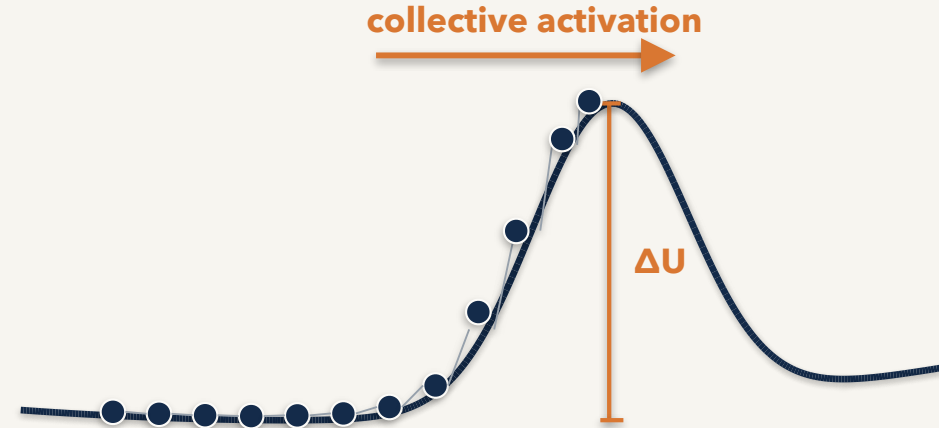
SINGLE PARTICLE



state described by one coordinate $x(t)$

Rare event: a single trajectory
surmounts the barrier

MANY INTERACTING PARTICLES • 1D



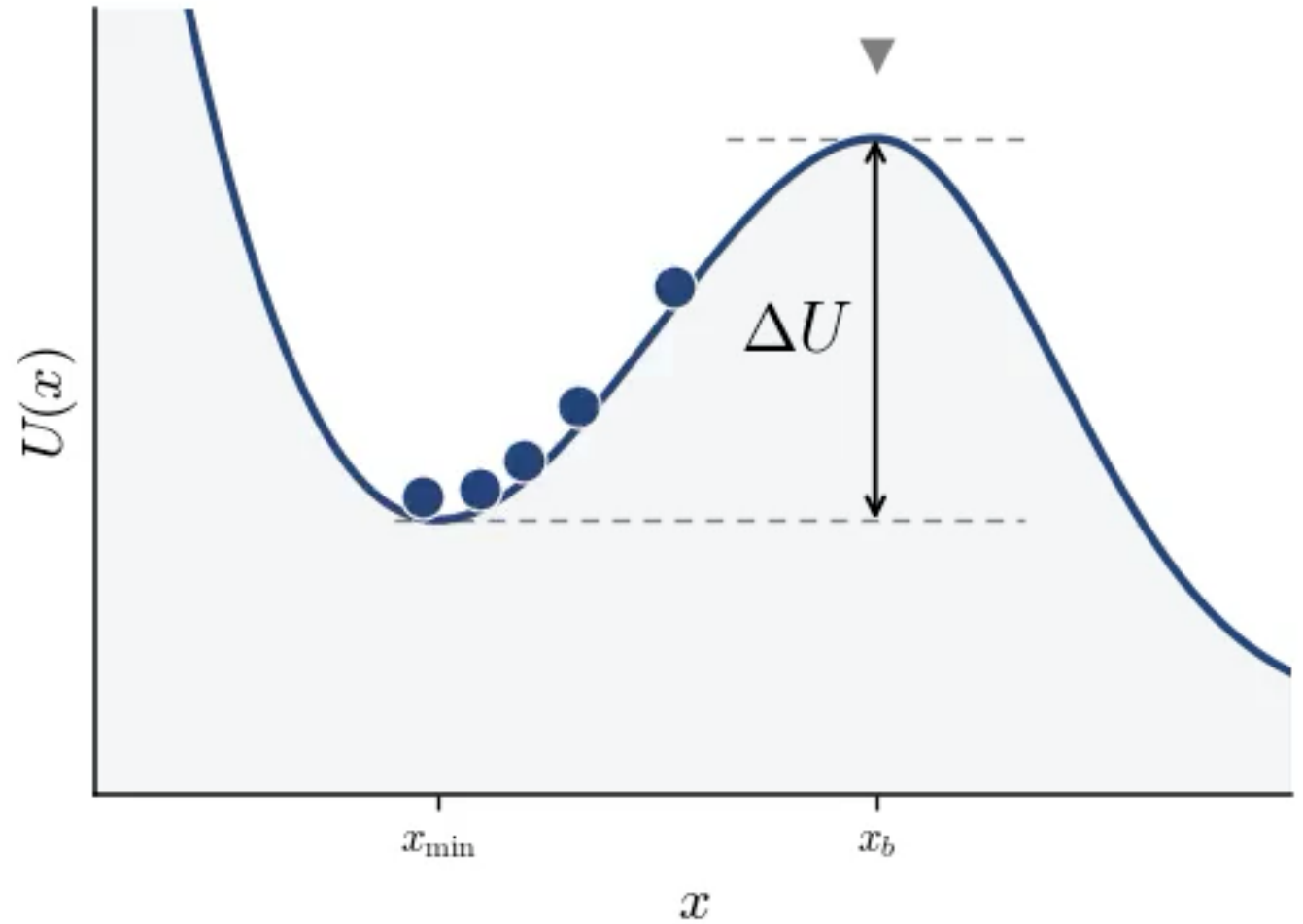
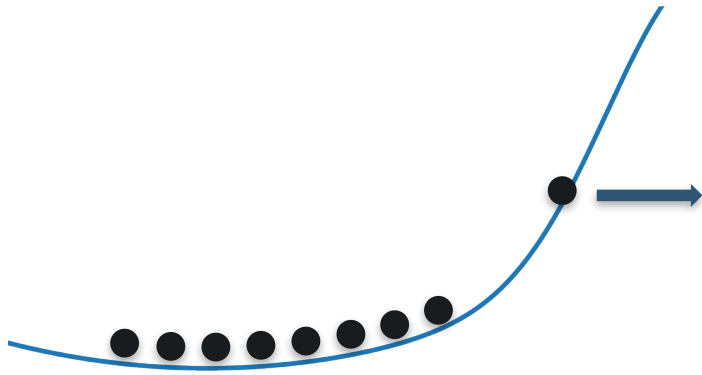
state described by N coordinates $\{x_1, \dots, x_n\}$

Rare event: a collective fluctuation
brings the leading particles over the barrier

One degree of freedom $\rightarrow$ many coupled degrees of freedom

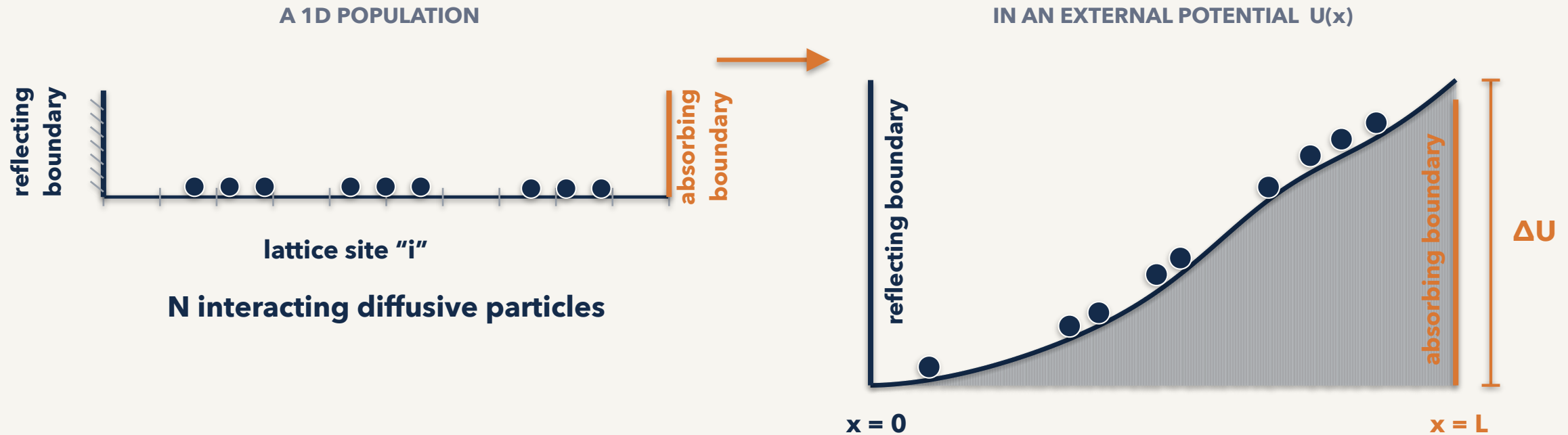
The barrier remains – but the activated object is now a collective configuration (?)

CENTRAL QUESTION: ESCAPE IN INTERACTING SYSTEMS?



THE SETUP

Many interacting diffusive particles move in a one-dimensional external potential



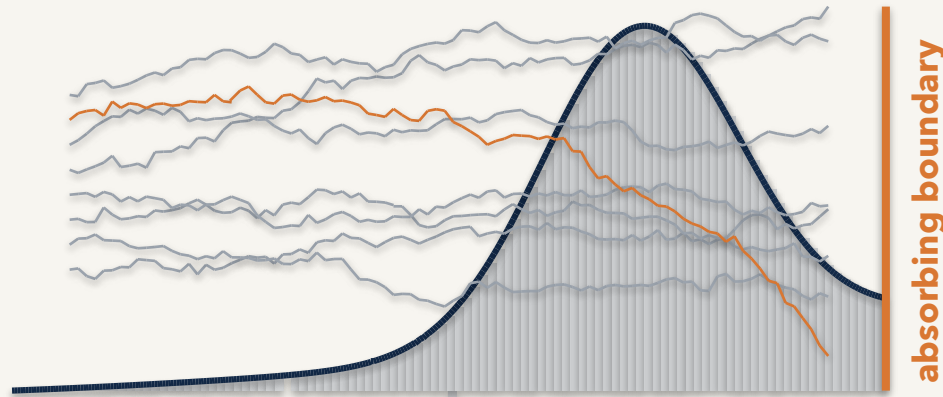
Large system size $L \rightarrow$ diffusive rescaling: position = i/L , time = t/L^2

What is the escape rate of the fastest particle?

THE NATURAL OBSERVABLE

How long does the population survive?

FROM TRAJECTORIES → FIRST PASSAGE



Each path is a possible history of the system

SURVIVAL PROBABILITY

$$Q_n(t) = P(T_1 > t, T_2 > t, \dots, T_n > t)$$

probability that no particle has reached $x = L$ by time t

Equivalently:

**sum of the probabilities of all trajectories
that avoid absorption up to time t**

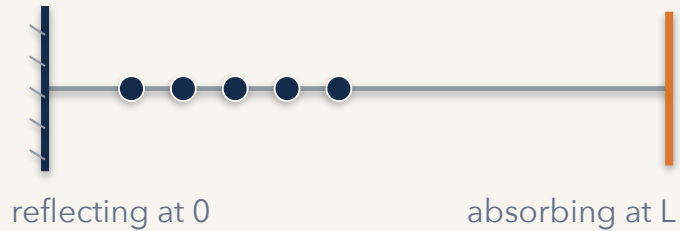
T_n = first-passage time of the n -th particle to the absorbing boundary

For many particles, the escape problem becomes complicated

THE NON-INTERACTING BASELINE

Before interactions: the many-particle problem is an extreme-value first-passage problem

N INDEPENDENT SEARCHERS



$$T_{\min} = \min(T_1, T_2, \dots, T_N)$$

The first particle to reach L
sets the population escape time

EXACT RELATIONS

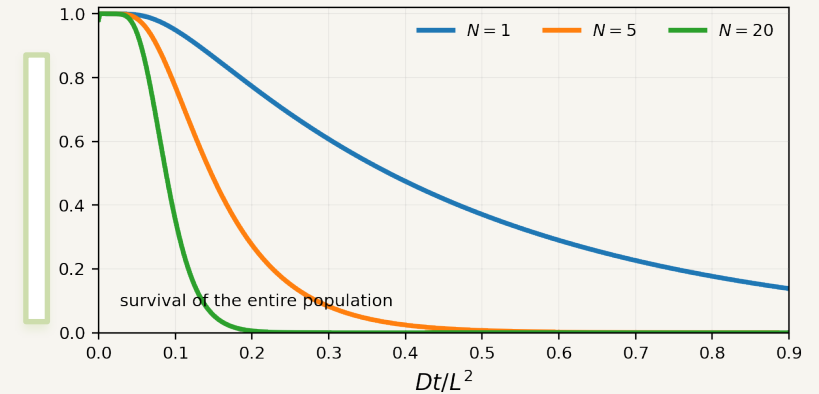
$$Q_N(t) = [Q_1(t)]^N$$

independence

$$\langle T_{\min} \rangle = \int_0^\infty Q_N(t) dt$$

MFPT of the fastest particle

SURVIVAL OF THE POPULATION



THE LONG-TIME ESCAPE RATE

$$\Phi_N \equiv \lim_{t \rightarrow \infty} \ln Q_N(t) = N\Phi_1$$

Activated speed/escape time $\Rightarrow$ an N-fold speed-up

WHAT ABOUT INTERACTING ONES?

FLUCTUATING HYDRODYNAMICS

Typical hydrodynamics tells us how the system normally evolves – but escape is a rare event

1 COARSE-GRAIN

particles $\rightarrow \rho(\mathbf{x},t), \mathbf{j}(\mathbf{x},t)$

Replace discrete positions by
local density and current

2 TYPICAL DYNAMICS

$$\partial_t \rho + \partial_x j = 0$$

$$J(\rho) = -D(\rho)\partial_x \rho - \chi(\rho)\partial_x U/D_0$$

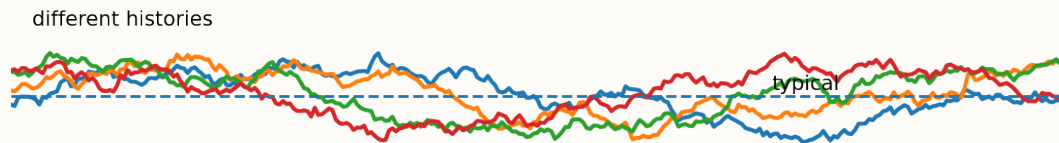
the most typical current

3 BUT ESCAPE IS RARE

**Typical evolution stays near
metastability**

It cannot tell us the probability
of crossing the barrier

ALLOW THE CURRENT "j" TO FLUCTUATE



Microscopic randomness appears as fluctuations of the coarse-grained current

SO WE ASK

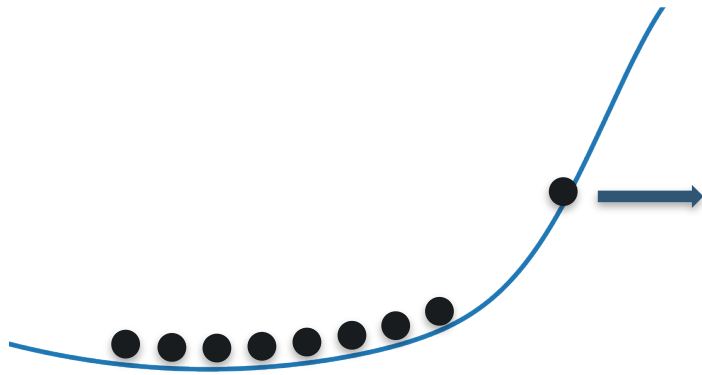
**Which fluctuating history
produces escape?**

$$P[\rho, j] \sim e^{-S[\rho, j]}$$

MFT assigns a probability cost to every
allowed density-current history

The escape problem becomes: find the least costly history that carries the system across the barrier

MACROSCOPIC FLUCTUATION THEORY



interacting particles in a confining potential

$\rho(x,t)$ – coarse-grained density $j(x,t)$ – current

$$\partial_t \rho + \partial_x j = 0$$

THE FLUCTUATING CURRENT HAS THREE PARTS

$$j = J(\rho) + \sqrt{2kT\chi/L}\xi(x,t)$$

DIFFUSION

density gradients drive spreading

$$-D(\rho)\partial_x \rho$$

EXTERNAL POTENTIAL

$$-\chi(\rho)\partial_x U$$

FLUCTUATIONS

microscopic randomness

$$\xi(x,t)$$

$$\langle \xi(x,t) \rangle = 0, \quad \langle \xi(x,t)\xi(x',t') \rangle = \delta(x-x')\delta(t-t')$$

A fluctuating hydrodynamic description of interacting diffusive particles

THE MSR PATH INTEGRAL

The probability to observe a fluctuation $\{\rho, j\}$ in the window $[0, t]$ has a large-deviation form:

$$\text{Prob}[\{\rho, j\}] \asymp e^{-S[\rho, j]}$$

Action

$$S[\rho, j] = \frac{L}{4D_0} \int dx \int dt \frac{[j - J(\rho)]^2}{\chi(\rho)}$$

Large L puts the calculation at its saddle point – the large-deviation structure

$$P[\{\eta\}] \sim e^{-\frac{1}{2D_0} \iint \eta^2 dx dt}$$

$$\eta = \sqrt{\frac{L}{2\chi(\rho)}} [j - J(\rho)]$$

no cost for the typical current

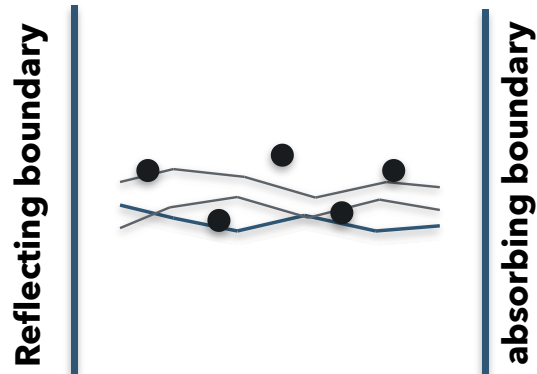
$$j = J(\rho) \Rightarrow S = 0$$

Any other current history costs a finite action

FROM FLUCTUATING HISTORIES TO SURVIVAL

Survival is a sum over all density-current histories that avoid the absorbing boundary

Many possible stochastic histories can contribute



But we sum only over histories that survive until time t

1 SINGLE PARTICLE SURVIVAL

$$Q(t) = \int_0^\infty dx \int_{x(0)=x_0}^{x(t)=x} \mathcal{D}[x(\tau)] e^{-\frac{1}{4D_0} \int_0^t d\tau \left[\frac{dx}{d\tau} + U'(x) \right]^2} \prod_{\tau=0}^t \Theta[x(\tau)]$$

2 MFT GIVES EACH HISTORY AN EXPONENTIAL WEIGHT

$$Q(t) = \int_{\text{surviving}} \text{Prob}[\{\rho, j\}] \Big|_{\text{BC}} ; \quad \text{Prob}[\{\rho, j\}] \asymp e^{-S[\rho, j]}$$

3 SURVIVAL TO ESCAPE RATE

$$Q(t) \asymp e^{-t \Phi} \quad \leftarrow \text{ESCAPE RATE/ INVERSE MFPT}$$

THE KEY IDEA: survival becomes a variational problem

Find the least unlikely density-current history compatible with not escaping

BOUNDARY CONDITIONS AND MASS CONSERVATION

The particles stay between 0 and 1: a reflecting wall at 0, an absorbing one at 1

$$J(\rho)|_{x=0} = 0$$

reflecting (RBC)

$$\rho|_{x=1} = 0$$

absorbing (ABC)

Every particle must still be there – mass is conserved

$$\int_0^1 dx \rho(x, t) = \frac{N}{L} = \bar{\rho}_0$$

Problem of history of smallest action – the least costly one under these BCs and conservation

$$Q(t) \asymp e^{-L \min_{\rho, j} \int dx dt \frac{(j - J(\rho))^2}{4D_0 \chi(\rho)}}$$

Extremely hard: two coupled
optimisations



Additivity principle

THE ADDITIVITY PRINCIPLE

Bodineau and Derrida, Phys. Rev. Lett. 92, 180601 (2024)

The optimal escape history becomes stationary – turning a space-time problem into a spatial one (this is not the STEADY STATE)

A stationary profile capable of producing a rare/atypical current

$$\rho^*(x, s) = \rho^*(x) \longrightarrow \partial_s \rho^* = 0 \implies \partial_x j^* = 0$$

optimal profile

additivity

reflecting boundary fixes the
constant current

$$j^*(0, s) = 0 \implies j^*(x, s) = 0$$

many admissible histories

Full optimisation is reduced

$$Q(t) \asymp e^{-L \min_{\rho, j} \int dx \, dt \frac{(j - J(\rho))^2}{4D_0 \chi(\rho)}}$$

SPACE-TIME → STATIC PROFILE

Only the density profile remains to be
optimized

$$Q(t) \asymp \exp \left[-\frac{tL}{4D_0} \min_{\rho(x)} \int_0^1 dx \frac{J(\rho(x))^2}{\chi(\rho(x))} \right]$$

- Optimal solution is dynamically stable against the time-dependent perturbations
- Now the escape rate is determined by an Euler-Lagrange problem for one optimal density profile

FROM THE OPTIMAL PROFILE TO THE EULER-LAGRANGE EQUATION

Once the current has vanished, only the stationary density profile remains to be determined

1 THE REDUCED VARIATIONAL PROBLEM

$$Q(t) \asymp \exp \left[-\frac{tL}{4D_0} \min_{\rho(x)} \int_0^1 dx \frac{J(\rho(x))^2}{\chi(\rho(x))} \right]$$

but the density is constrained by particle conservation:

$$\int_0^1 dx \rho(x) = \rho_0$$

↓ Lagrangian

$$Q(t) \asymp \exp \left[-\frac{tL}{4D} \min_{\rho(x)} \int_0^1 dx \mathcal{L}(\rho, \partial_x \rho) \right]$$



2 MAKE THE NONLINEAR PROBLEM TRACTABLE

Introduce a Lagrange multiplier Λ and minimize

$$\mathcal{L} = \frac{J(\rho)^2}{\chi} - 4\Lambda(\rho - \bar{\rho}_0)$$



Escape rate $\Phi = \frac{D_0 L}{4} \min_{\rho(x)} \int dx \mathcal{L}(\rho, \partial_x \rho)$

THE MANY-BODY ESCAPE RATE → ONE CONSTRAINED BOUNDARY-VALUE PROBLEM FOR THE OPTIMAL DENSITY

EL and F-transformation

Euler-Lagrange equation for the optimal profile

$$\frac{\partial \mathcal{L}}{\partial \rho} - \frac{d}{dx} \frac{\partial \mathcal{L}}{\partial (\partial_x \rho)} = 0$$

Euler-Lagrange condition $\rightarrow$ nonlinear eigenvalue problem

the F-transformation

$$F(\rho) = \int_0^\rho dz \frac{D(z)}{2\sqrt{\chi(z)}}$$

T. Agranov and B. Meerson, Phys. Rev. Lett. 120, 120601 [2018]
Meerson, Vilenkin and Krapivsky Phys. Rev. E. 90, 022120 [2014]

Escape rate

$$\Phi = D_0 L \int dx J_F^2$$

$$\mathcal{N}[F] = \Lambda W[F]$$

Very hard to compute

Rescaled current $J \rightarrow J_F$

$$J_F = \partial_x F + \frac{1}{2} \chi^{1/2}(F) \partial_x U / D_0$$

Boundary conditions $J_F|_{x=0} = F|_{x=1} = 0$

REVISITING NON-INTERACTING BM REGIME

For non-interacting particles

$$D = 1, \chi = \rho$$

the F-transformation

$$\rho = F^2$$

Linear eigenvalue problem

$$\mathcal{N}[F] = \Lambda W[F] \rightarrow \hat{H}_{FP} F = \Lambda F$$

Solve the eigenvalue problem and find the ground state

$$\hat{H}_{FP}/D_0 = -\partial_{XX} + \frac{1}{4} \left(\frac{\partial_X U}{D_0} \right)^2 + \frac{\partial_{XX} U}{2D_0}$$

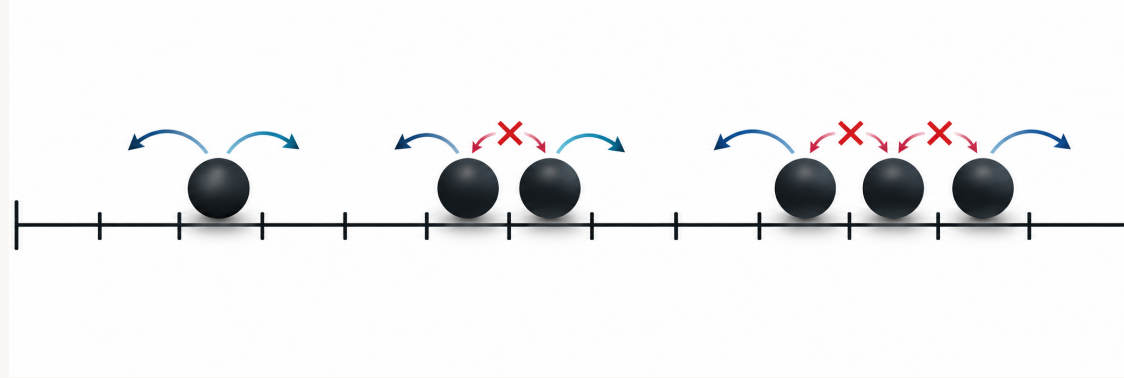
Escape rate

$$Q(t) \asymp e^{-t N \Lambda}$$

Where we are at

- Macroscopic Fluctuation theory
- Stationary optimal profile
- Constrained minimization with boundary conditions
- F-transformation with boundary conditions
- Nonlinear eigenvalue problem
- Exact solution (limited); numerically solvable

Symmetric Exclusion Process



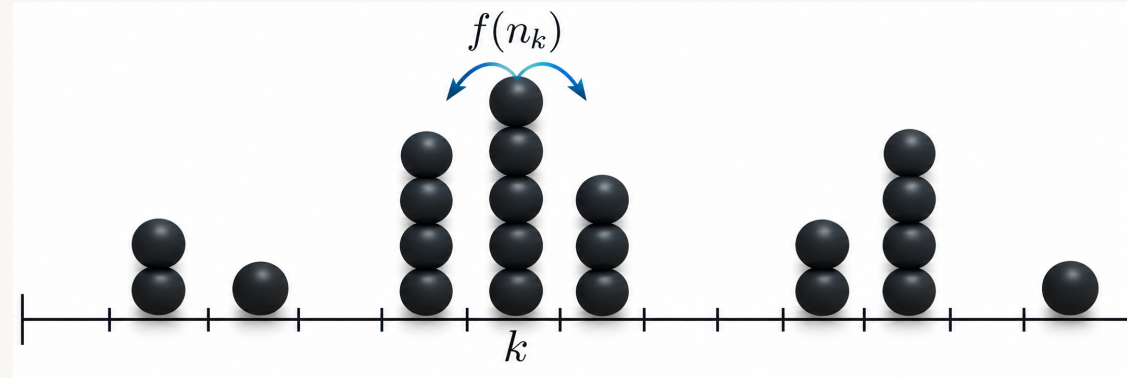
Hard-core exclusion: Each lattice site can host at most one particle $n_k \in (0,1)$; particles hop only to an empty nearest-neighbour site.

Symmetric hopping: Left/right hopping occur with equal rates $\Rightarrow$ no net drift and diffusive transport.

Conservation & hydrodynamics: Particle number is conserved in the bulk, and on large scales

$$D(\rho) = 1, \chi(\rho) = \rho(1 - \rho)$$

Zero Range Process



No exclusion: Multiple particles can occupy the same site, $n_k = 0, 1, 2, \dots$

Zero-range interaction: A particle leaves site k with a rate that depends only on the occupation n_k

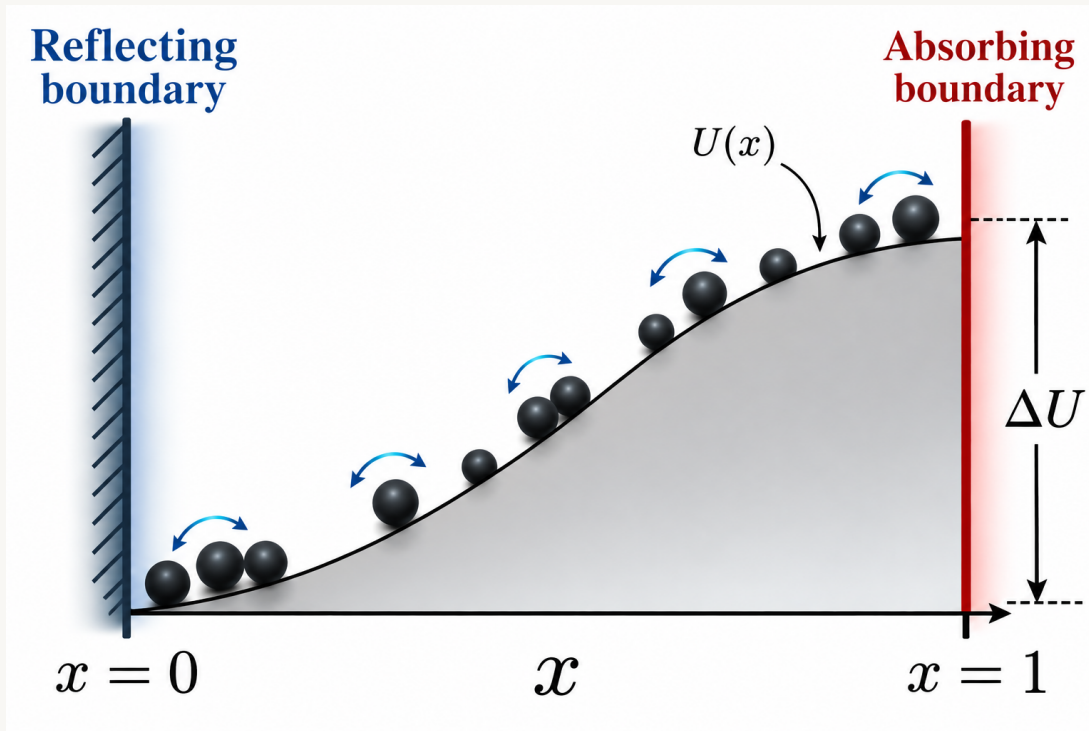
$$n_k \rightarrow n_k - 1, \quad n_{k+1} \rightarrow n_{k+1} + 1 \quad \text{at rate } f(n_k)$$

Product-form steady state: exactly tractable steady state

Condensation: Macroscopic occupation

controlling the particle density in the grand-canonical ZRP

$$D(\rho) = \partial_\rho \lambda, \chi(\rho) = \lambda; \quad \lambda = \text{fugacity}$$



$$U(x) = \Delta U x \text{ (linear)}$$

$$U(x) = \Delta U x^2 \text{ (harmonic)}$$

$$U(x) = \frac{1}{2} \Delta U (1 - \cos(\pi x)) \text{ (cosine)}$$

CENTRAL RESULT

The Canonical AL

$$Q(t) \asymp \exp [-t \Phi]$$

Weak noise + Large barrier limit

$$D_0 = k_B T \ll \Delta U$$



$$\Phi \asymp e^{-\Delta U/D_0}$$



The Generalised AL

- interacting diffusing particles
- monotonically increasing potential $U(x)$
- fixed initial mean density $\bar{\rho}_0 = N/L$

$$\Phi \asymp e^{-\Delta U g(\bar{\rho}_0)/D_0}$$

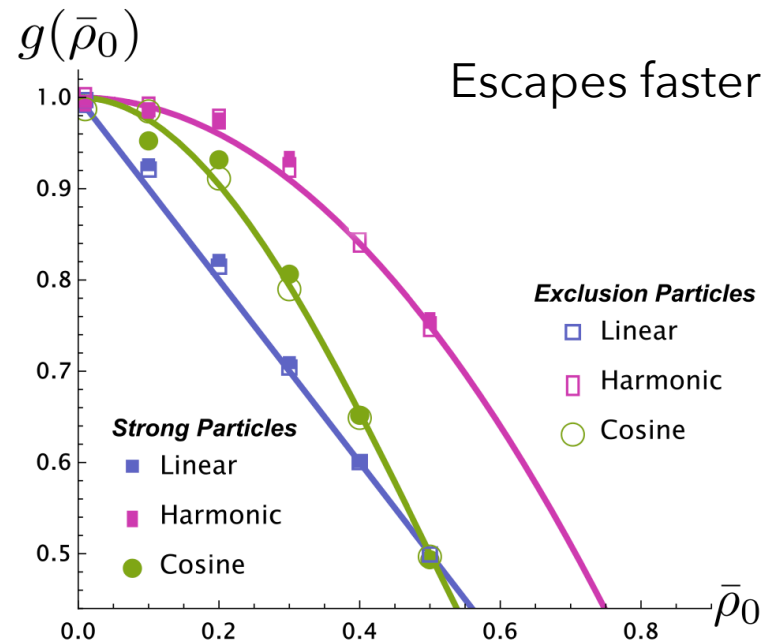


New "Effective" Barrier

NUMERICS

EXCLUDED VOLUME UNIVERSALITY

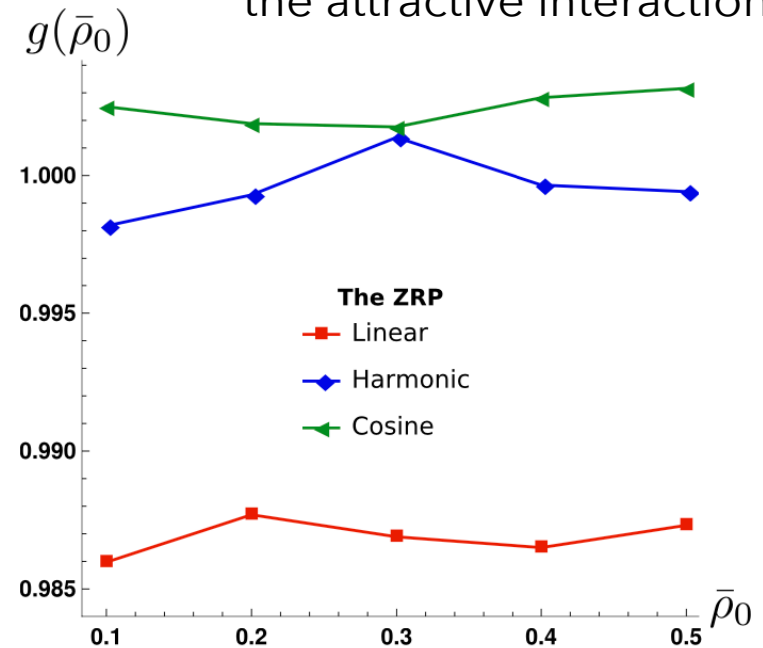
$$U_{\text{top}} = U(x = \bar{\rho}_0) \implies g < 1$$



ARRHENIUS UNIVERSALITY

$$U_{\text{top}} = 0 \implies g = 1$$

No slowing down due to the attractive interaction



NUMERICAL SOLUTION OF THE NON-LINEAR EIGENVALUE EQUATION WITH BOUNDARY CONDITIONS

INTERPRETATION

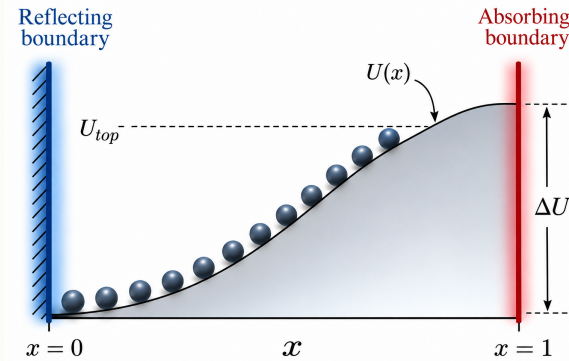
TWO UNIVERSALITY CLASSES

$$\Phi \asymp e^{-\Delta U g(\bar{\rho}_0)/D_0}$$

$$g = 1 - U_{\text{top}}/\Delta U$$

highest energy a particle can attain in the minimum energy configuration

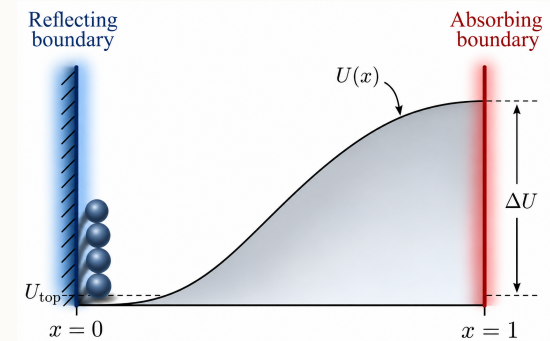
EXCLUDED VOLUME UNIVERSALITY



$$U_{\text{top}} = U(x = \bar{\rho}_0) \implies g < 1$$

Tight packing and exclusion leads to an effective barrier seen by the last particle

ARRHENIUS UNIVERSALITY

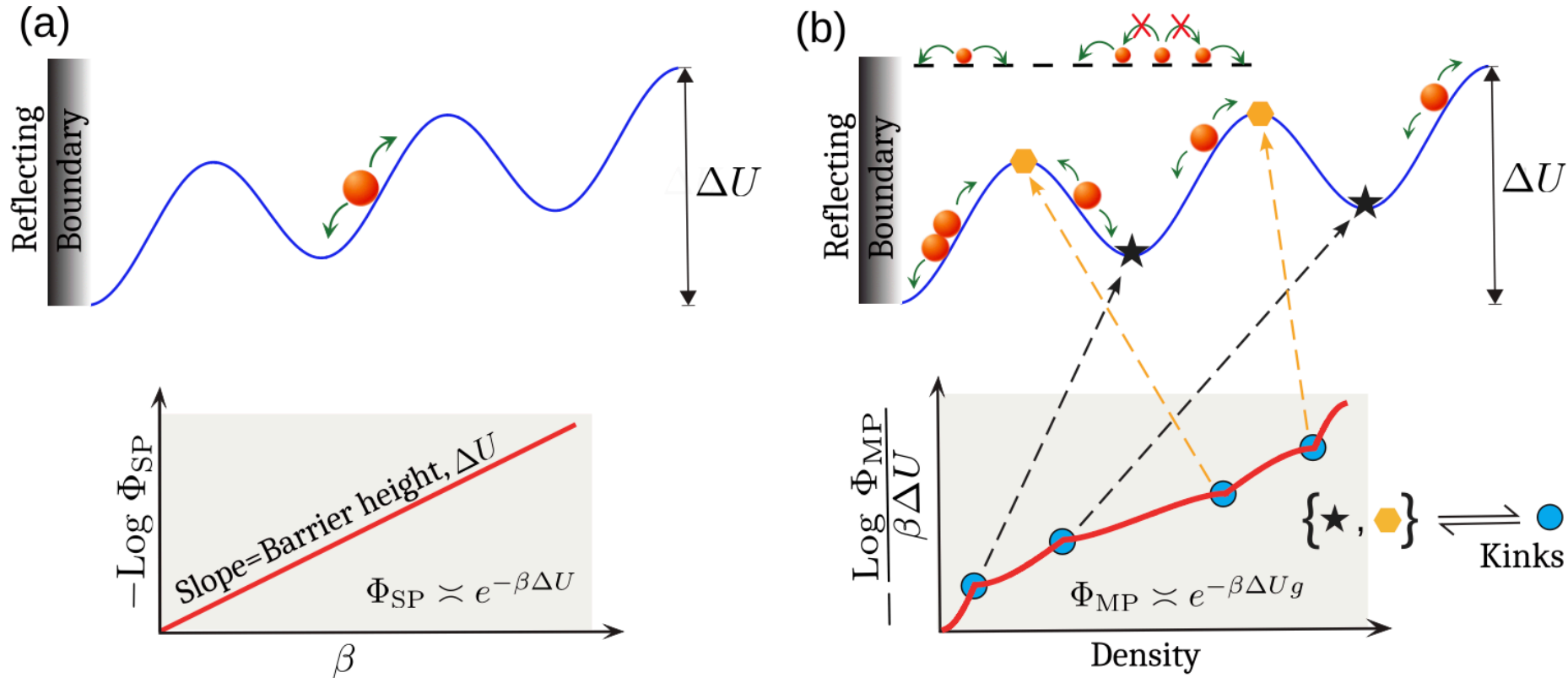


$$U_{\text{top}} = 0 \implies g = 1$$

No slowdown in the escape, attractive interactions imply that the minimum energy configuration is attained when all the particles bunch at the potential minimum

The key issue here is with excluded volume or not, does not depend on the nature of the interactions

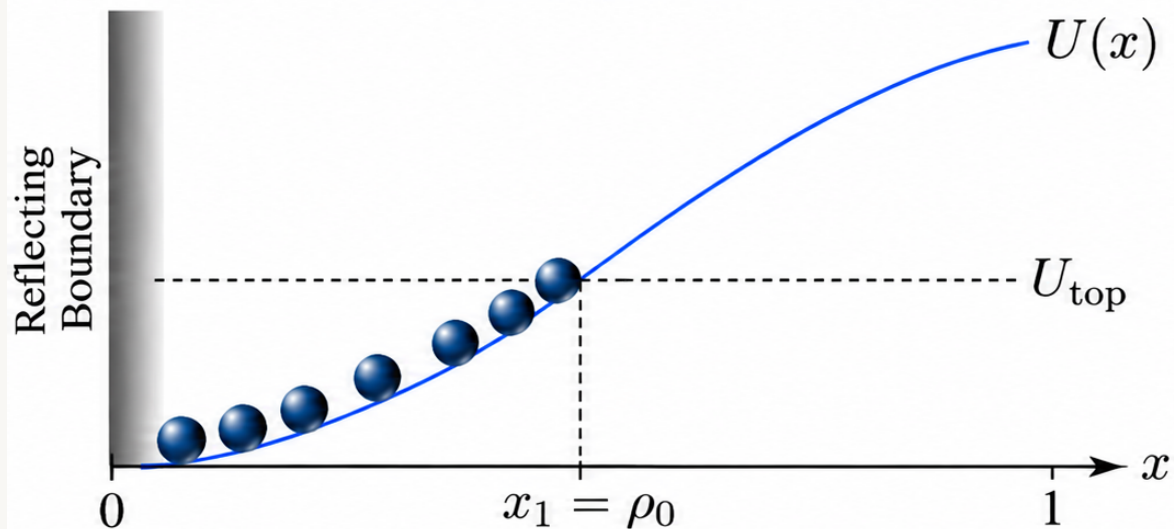
INFERENCE USING GENERALISED AL: A SIMPLE STEP



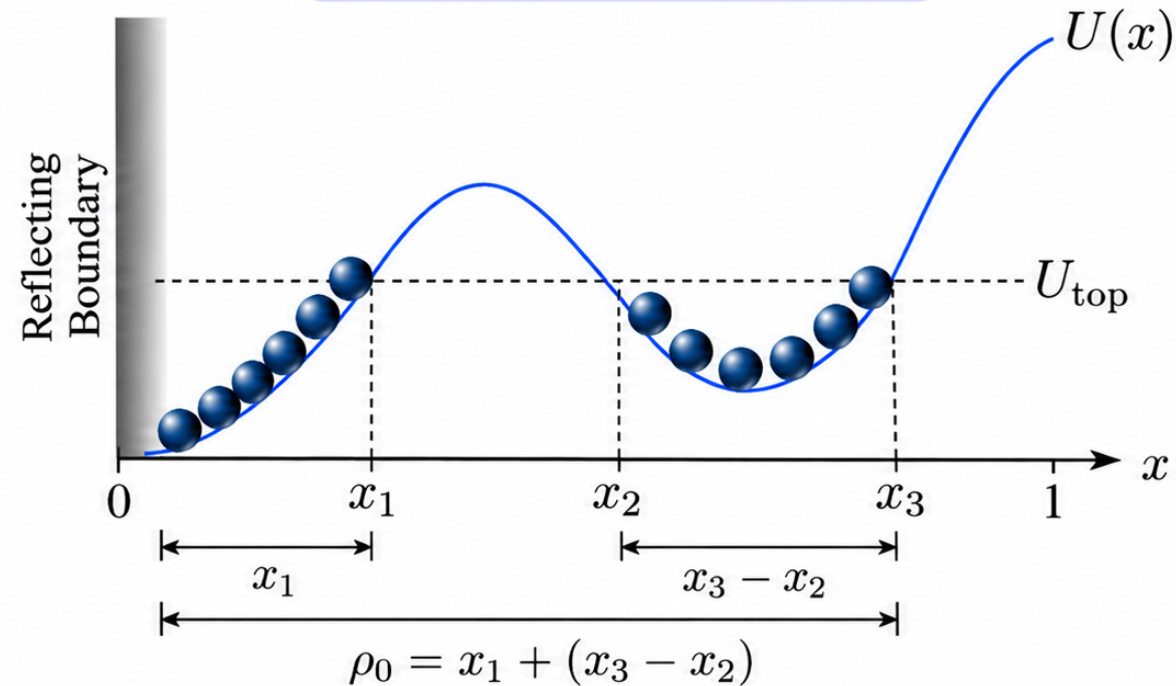
Poster by Vishwajeet

It is the local minima and maxima of the potential trap that introduce kinks in g for the non-monotonous potentials

(a) Monotonic potential



(b) Non-monotonic potential



Potential	Lowest-energy region	Last-particle energy	Relation
Monotonic $U(x)$	$[0, \rho_0]$	$U(\rho_0)$	$U_{\text{top}} = U(\rho_0)$
Non-monotonic $U(x)$	$[0, x_1] \cup [x_2, x_3]$	$U(x_1) = U(x_2) = U(x_3) = U_{\text{top}}$	$U_{\text{top}} \neq U(\rho_0)$

Minimum-energy principle: occupy the lowest-energy sites first

$$g(\rho_0) = 1 - U_{\text{top}}(\rho_0)/\Delta U \text{ but } U_{\text{top}} \neq U(x = \rho_0)$$

$$\rho_0 = \int dx \Theta[U_{\text{top}} - U(x)]$$

Emergence of "kinks"

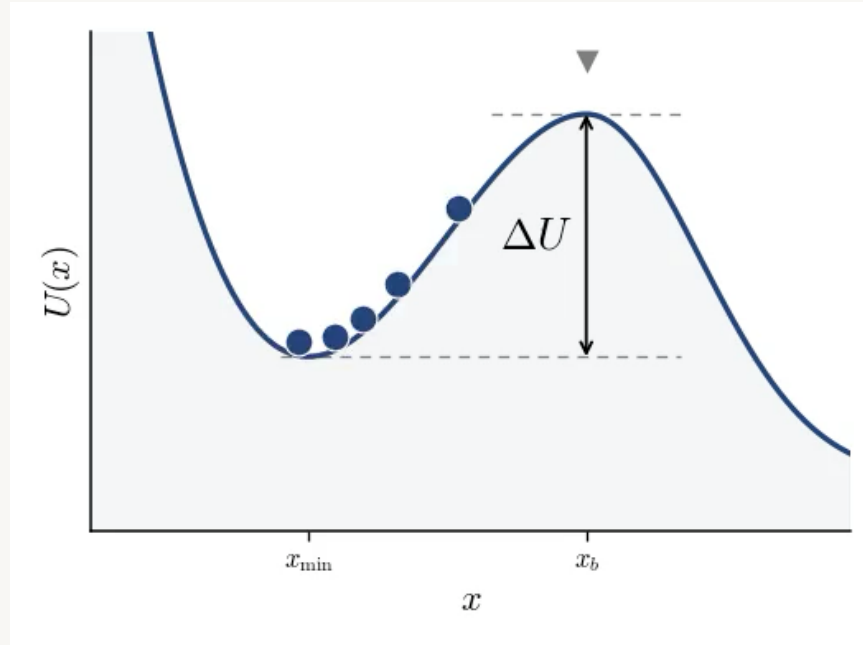
SUMMARY & CONCLUDING REMARKS

- We have discovered a new AL universality class for interacting diffusive systems.
- Particle models with excluded volume exhibit a decrease in g leading to a facilitated escape from the potential.
- Importantly g is independent of the interaction.
- Whenever excluded volume effects are not present, we reach quite surprisingly and non-trivially to an effective single particle problem.
- Thus, the canonical AL applies for processes without excluded volume effects.
- Albeit its technical simplicity and intuitively appealing physical interpretations, any attempts to generalize the insight gained from single particle AL to many particles with arbitrary interactions remains exorbitantly challenging.

OPEN DIRECTIONS

- Generalise AL to include arbitrary potential landscape, possibly also to higher dimensions
- AL for multi-species particles, where D, χ become matrices.
- Can such inter-species interactions speed up the escape rate of a complex activation process?
- Ballistic particles and escape properties? PRL 135 (22), 227101 [2025], PRL **137**, 127102 [2026]
- Full-scale simulations and shed light on the ordered statistics, tagged particle escape
- Experiments on channels are available to test our theory, a critical issue seems to be the variation of the barrier
- Can AL be used to infer landscape more rigorously?

ACKNOWLEDGEMENTS



विज्ञान एवं प्रौद्योगिकी विभाग
DEPARTMENT OF
SCIENCE & TECHNOLOGY