FROM CELL MEMBRANES TO ULTRACOLD GASES: CLASSICAL AND QUANTUM DIFFUSION IN INHOMOGENEOUS MEDIA

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Outlook

A. Classical

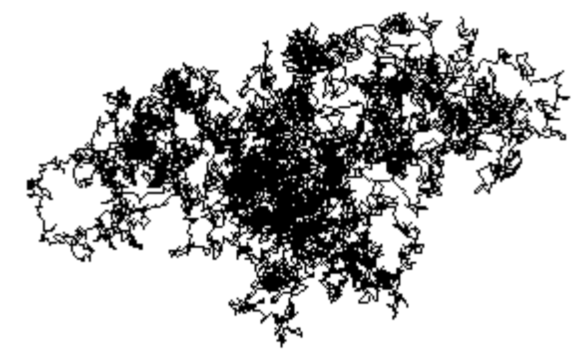
- Anomalous diffusion in biological systems
- Kinetic Ising Models

B. Quantum

- Quantum Kinetic Ising Models
- Quantum Brownian Motion

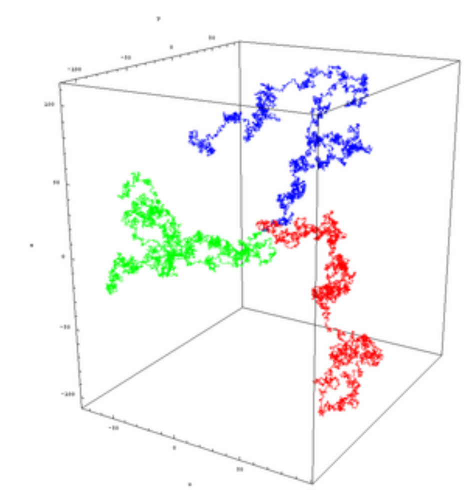
Ordinary Random Walk

Time-averaged mean squared displacement along a single trajectory:



$$\text{T-MSD}(t_{lag} = m\Delta t) = \frac{1}{N-m} \sum_{i=1}^{N-m} \big(x\,(t_i + m\Delta t) - x\,(t_i)\big)^2$$

Ensemble-averaged mean squared displacement over J trajectories:

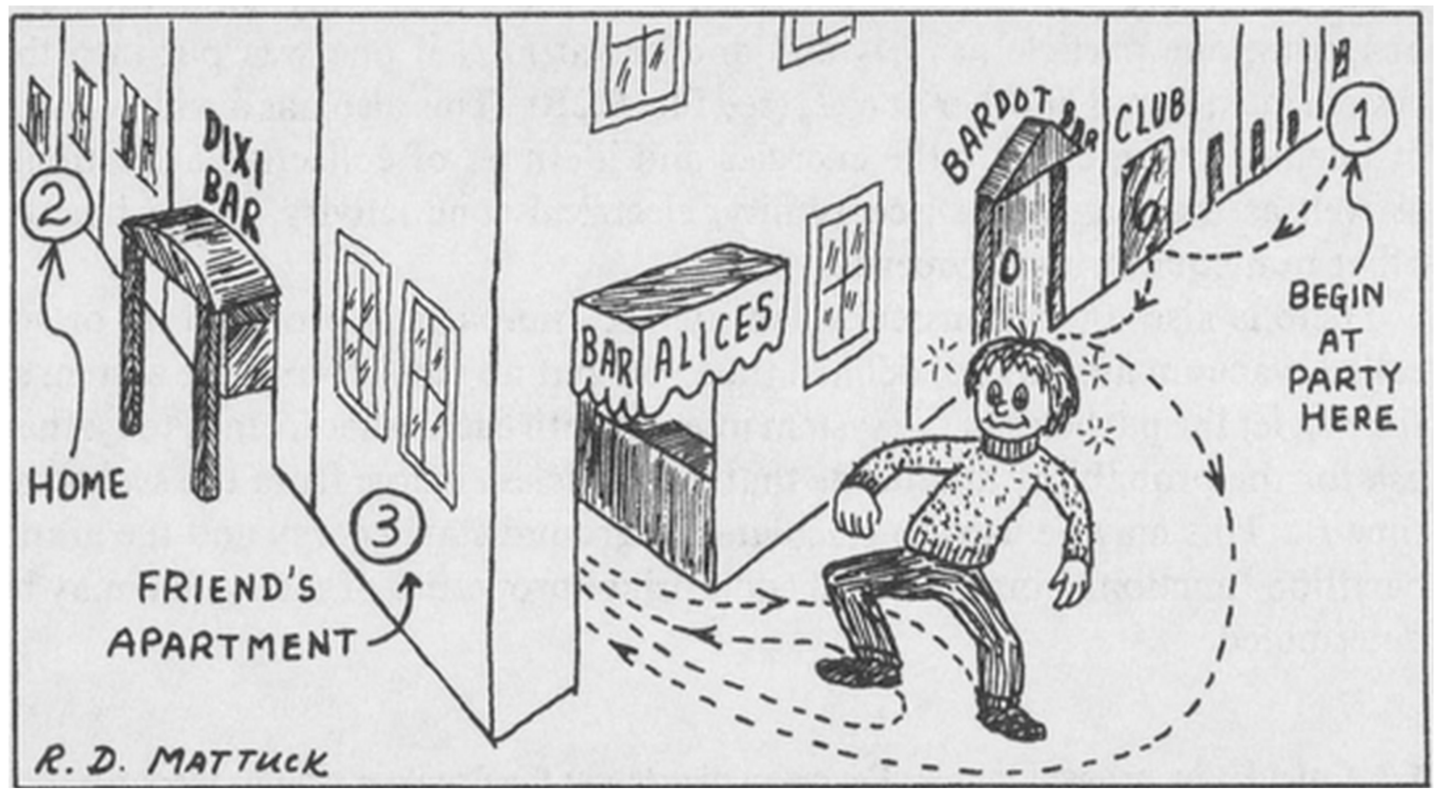


$$\text{E-MSD}(t_{lag} = m\Delta t) = \frac{1}{J} \sum_{j=1}^{J} \big(x_j\,(t_i + m\Delta t) - x_j\,(t_i)\big)^2$$

An ordinary RW is

- diffusive: MSD~t^{β}, with β=1
- ergodic: T-MSD and E-MSD coincide at long times
- stationary: MSD independent of the total observation time (at large times)

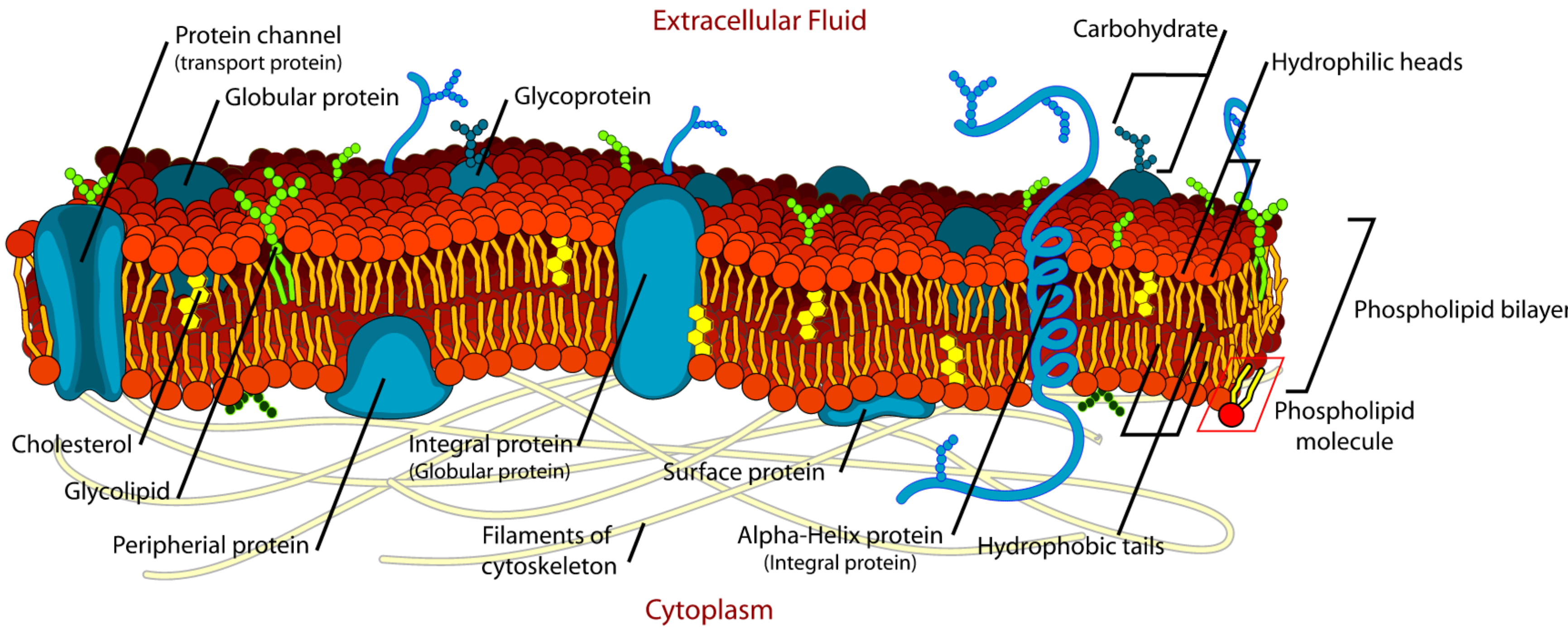
Diffusion in structured media



A random walker may be strongly affected by:

- repeated interactions
- transient binding
- clustering
- crowding
- multi-scale, or scale-free, disorder

Live cell membrane



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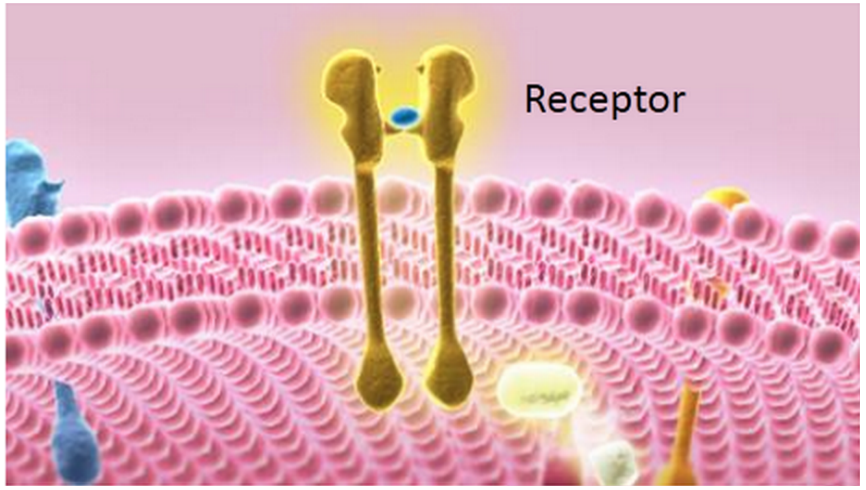
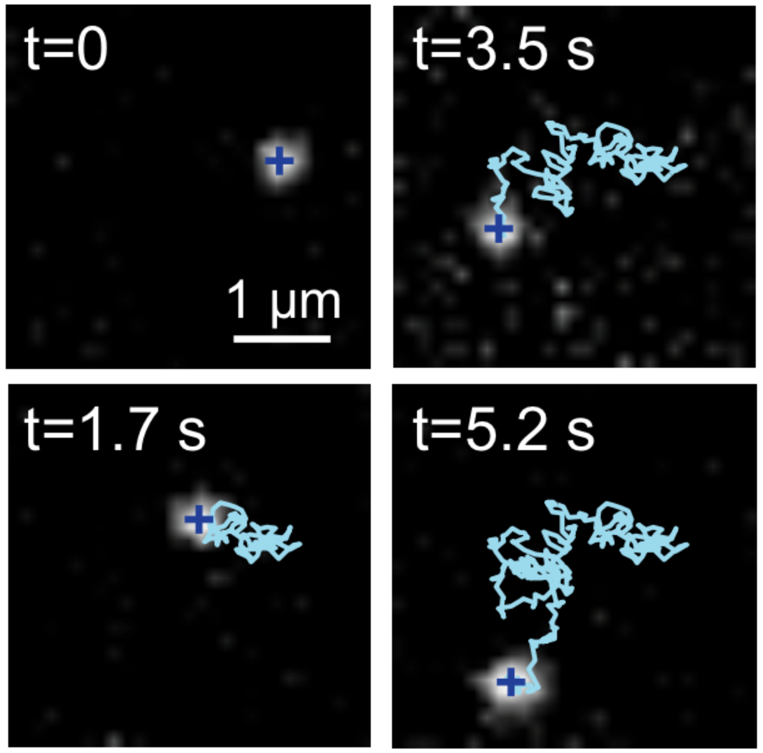
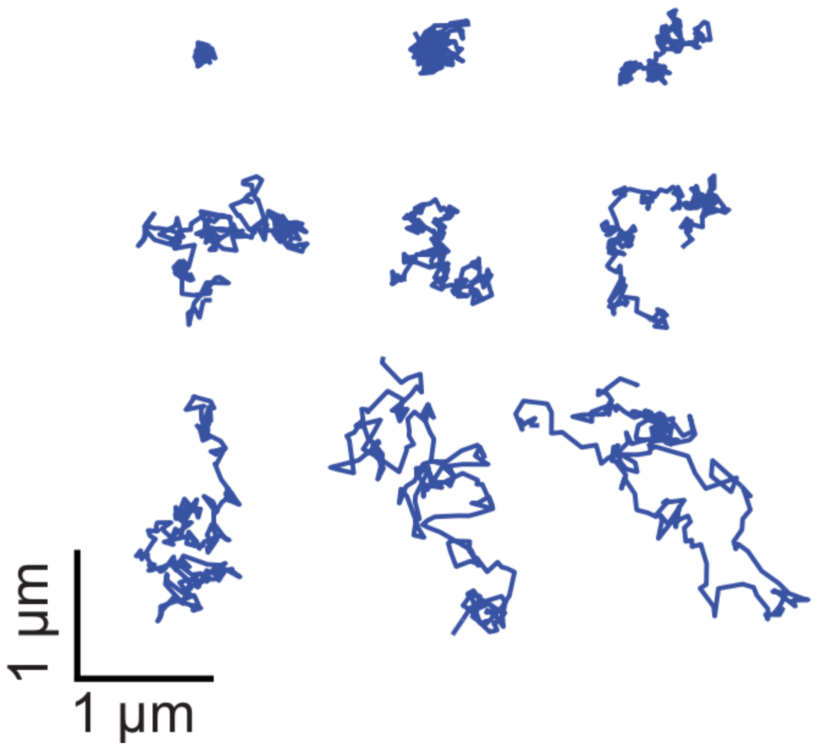
Trans-membrane receptors

Single particle tracking of pathogen-recognizing receptors on live cellular membranes

(M. García-Parajo's group @ ICFO)





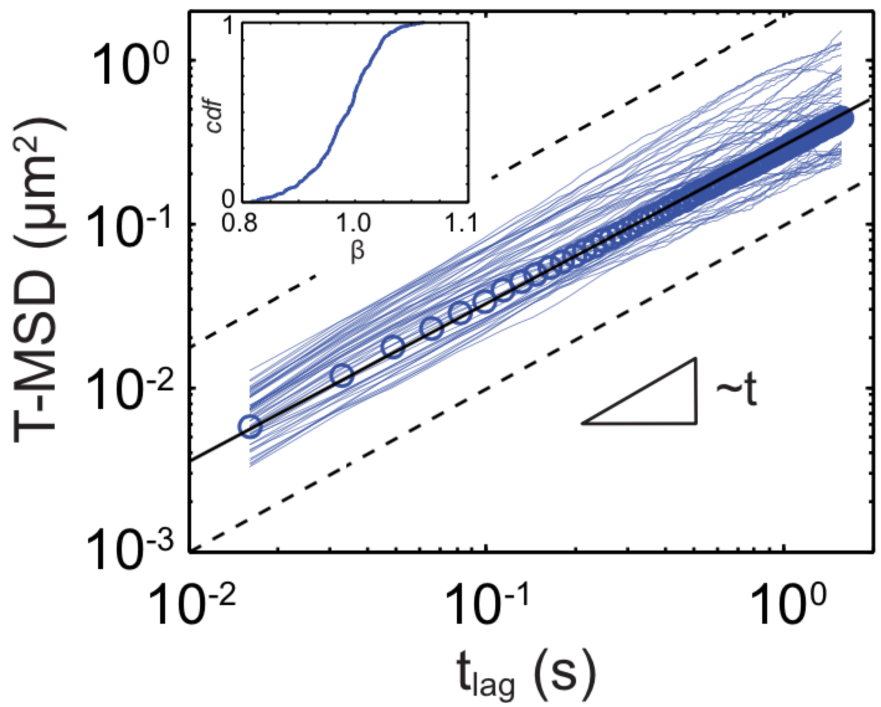


60 frames/s
20nm position accuracy

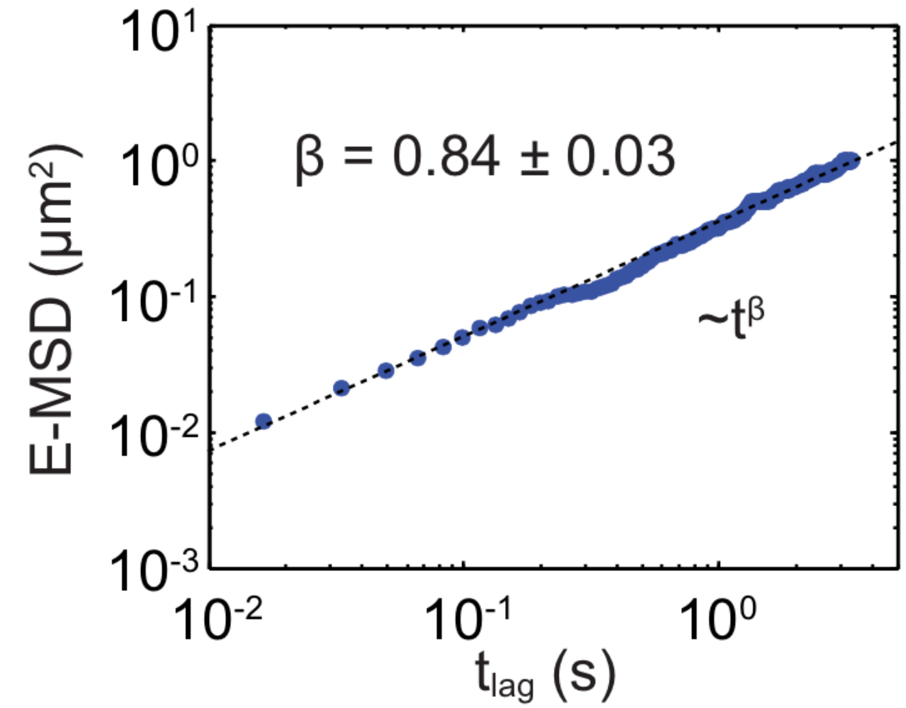
Manzo, Torreno-Pina, PM, Lapeyre, Lewenstein & García-Parajo, Phys. Rev. X (2015)

Sampling of J=600 trajectories

Time-averaged MSD

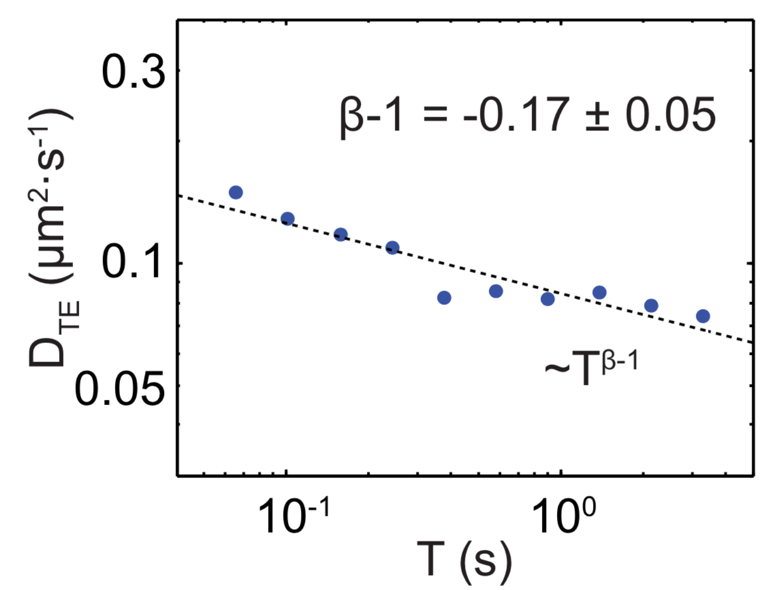


Ensemble-averaged MSD



Different scaling of T-MSD and E-MSD ➟ **weak ergodicity breaking!**

Time&Ensemble averaged MSD: $\text{TE-MSD} \sim D_{\text{TE}}(T) \cdot t_{lag}$



The TE-MSD depends on the total observation time T ➟ **non-stationary!**

Continuous-Time Random Walk

- CTRW: a fat-tailed distribution of waiting times $\sim t^{-1-\beta}$ with $\beta \leq 1$ (so that $\langle t_{wait} \rangle = \infty$) induces non-stationary (thus non-ergodic) subdiffusion with E-MSD$\sim t^{\beta}$ and TE-MSD$\sim D_{TE}(T)^{*} t_{lag}$, with $D_{TE} \sim T^{\beta-1}$

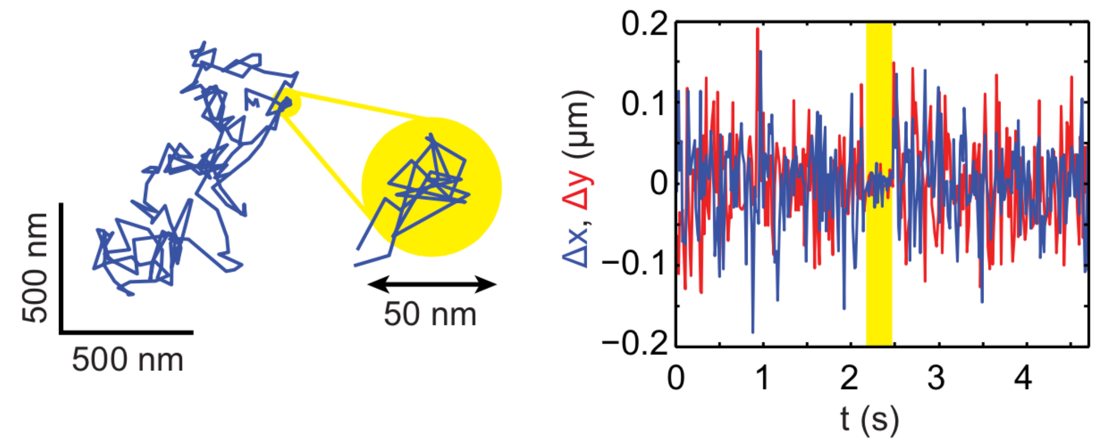
- Widely used model for transport in disordered media (initially developed for amorphous solids)

Montroll & Weiss, 1965; Montroll & Scher, 1973

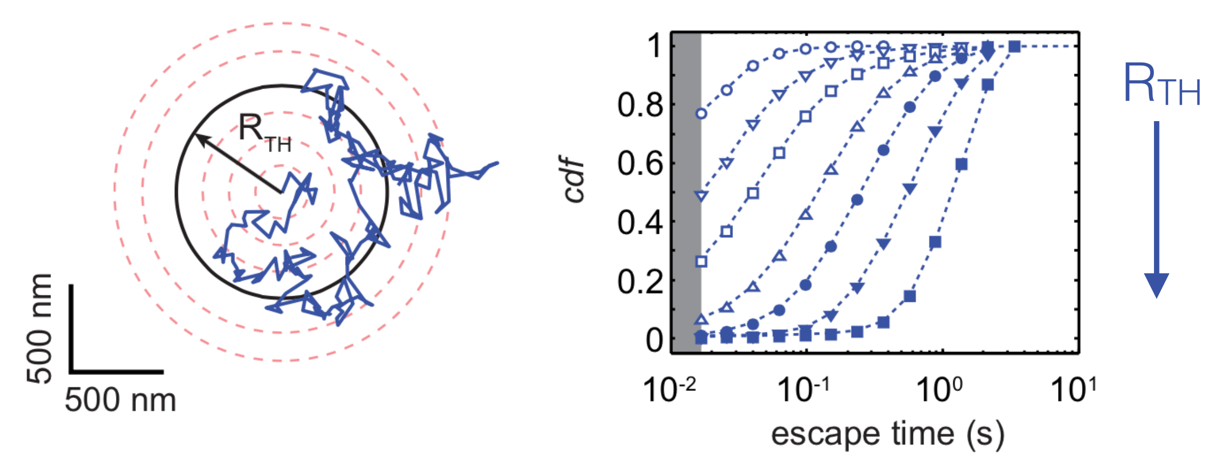
- However, *are trapping events present in the ICFO experiment?*

only 5% of the trajectories contain events compatible with transient trapping

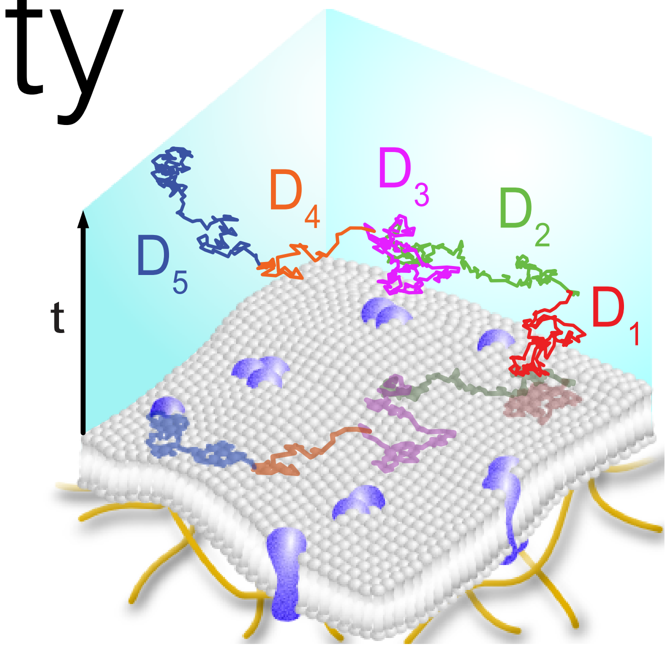
and excluding these trajectories yields a very similar E-MSD exponent β



- For CTRW, the long-time dynamics is dominated by anomalous trapping events, so that the escape-time distribution at long times becomes independent of the trapping radius R_{TH}



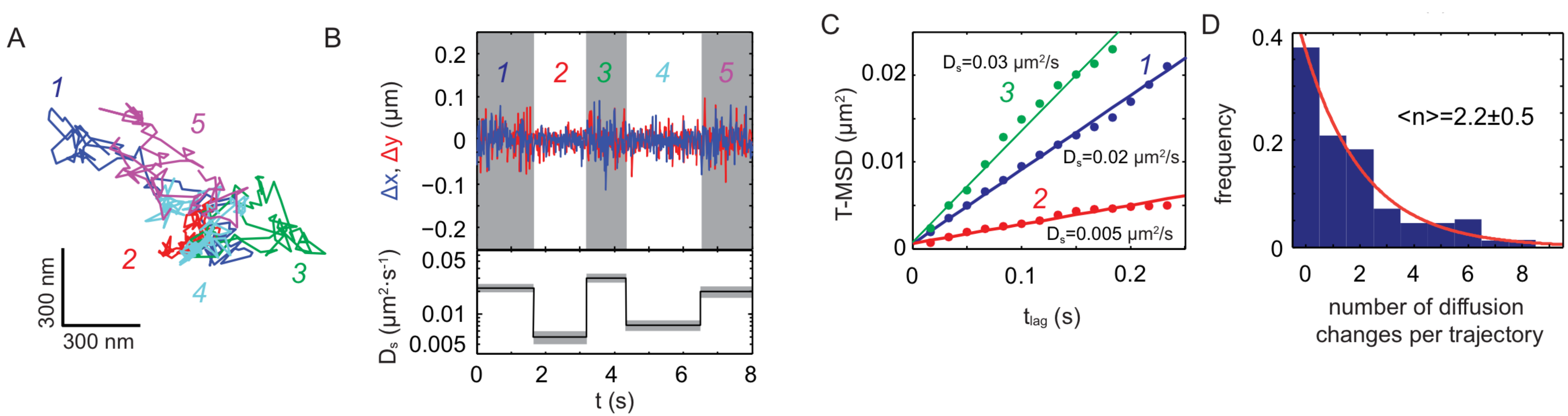
Strongly varying diffusivity



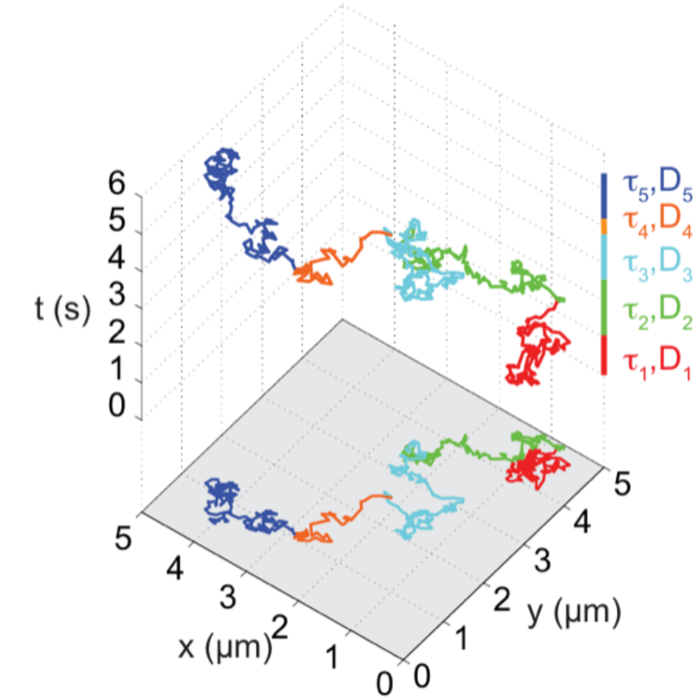
- Maps of receptor motion on the cell membrane highlight the presence of patches with strongly varying diffusivity

- Many possible reasons: crossing regions of low/high viscosity, transient binding, clustering, …

- Employ a likelihood-based Bayesian algorithm to detect *time-dependent changes of diffusivity within a single trajectory*:



Theoretical model



- Ordinary Brownian motion with a diffusivity that varies randomly, but it's constant on time intervals with random duration (or patches with random sizes)

- Assume a distribution of diffusion coefficients $P_D(D) \sim D^{\sigma-1} e^{-D/b}$

  power law at small D
  fast decay at large D

  and a conditional distribution of transit times $P_\tau(\tau|D) \sim D^\gamma e^{-\tau D^\gamma/k}$

  mean transit time ~$D^{-\gamma}$
  each area has radius r~$(\tau D)^{-1/2}$

- Three possible regimes:

(0) γ<σ: the long-time dynamics is compatible with regular Brownian motion (β=1)

(I) σ<γ<σ+1: the average transit-time diverges ➟ non-ergodic sub-diffusion (β=σ/γ)

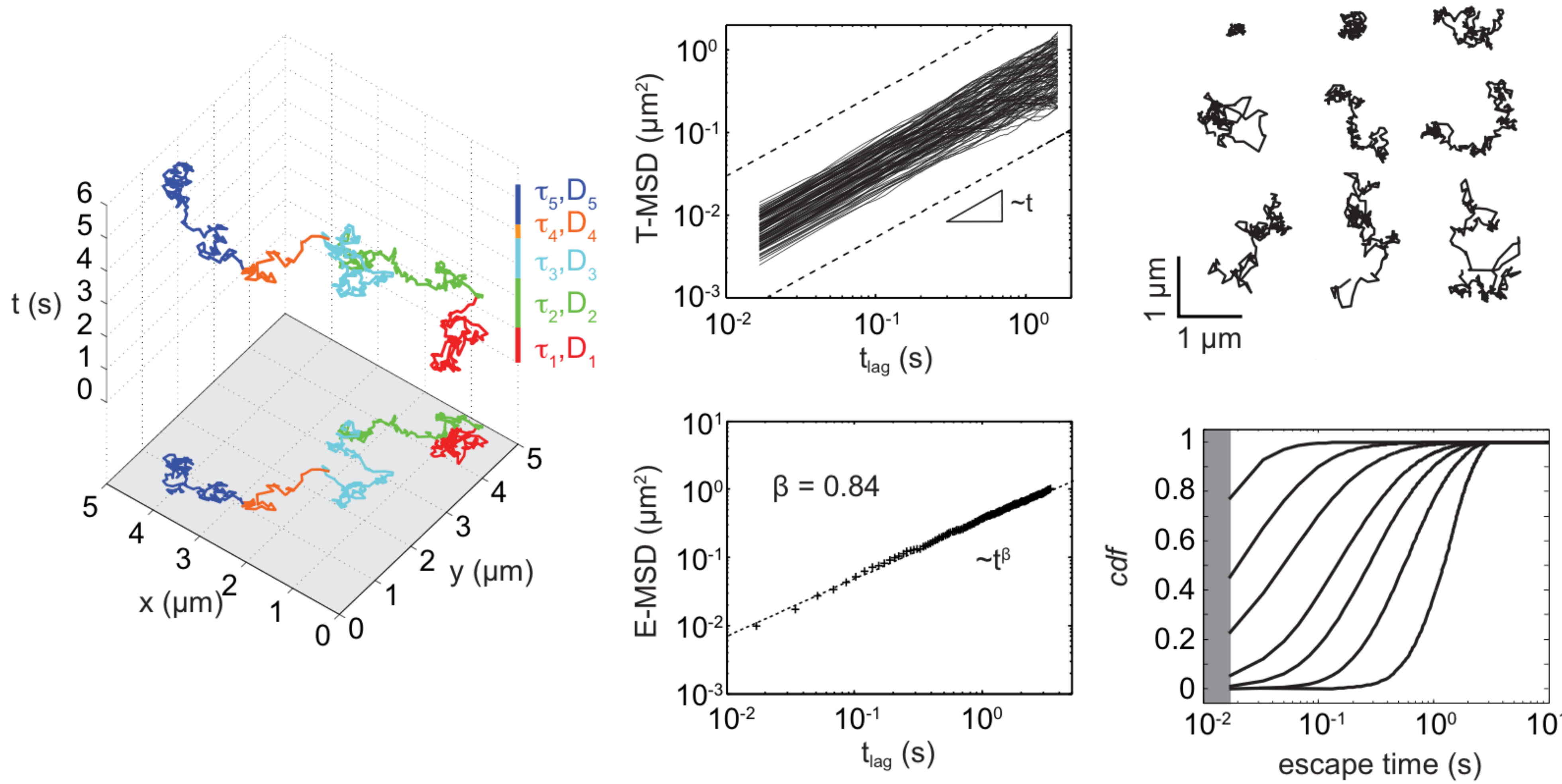
(II) γ>σ+1: both <τ> and $<(r_{area})^2>$ diverge ➟ non-ergodic sub-diffusion (β=1-1/γ)

PM, Manzo, Torreno-Pina, García-Parajo, Lewenstein & Lapeyre, Phys. Rev. Lett. (2014)

Comparison with experiments

Simulation of
WT dynamics
σ=1.16
γ=1.38
regime **(I)**

non-ergodic subdiffusion
with β=σ/γ=0.84



Instead, mutated receptors with impaired function (Δ_{rep}) may be best simulated with γ<σ, i.e., they perform usual ergodic and diffusive Brownian motion

<u>Transport properties strongly linked to molecular function</u>

Manzo, Torreno-Pina, PM, Lapeyre, Lewenstein & García-Parajo, Phys. Rev. X (2015)

Include receptor/membrane interactions?

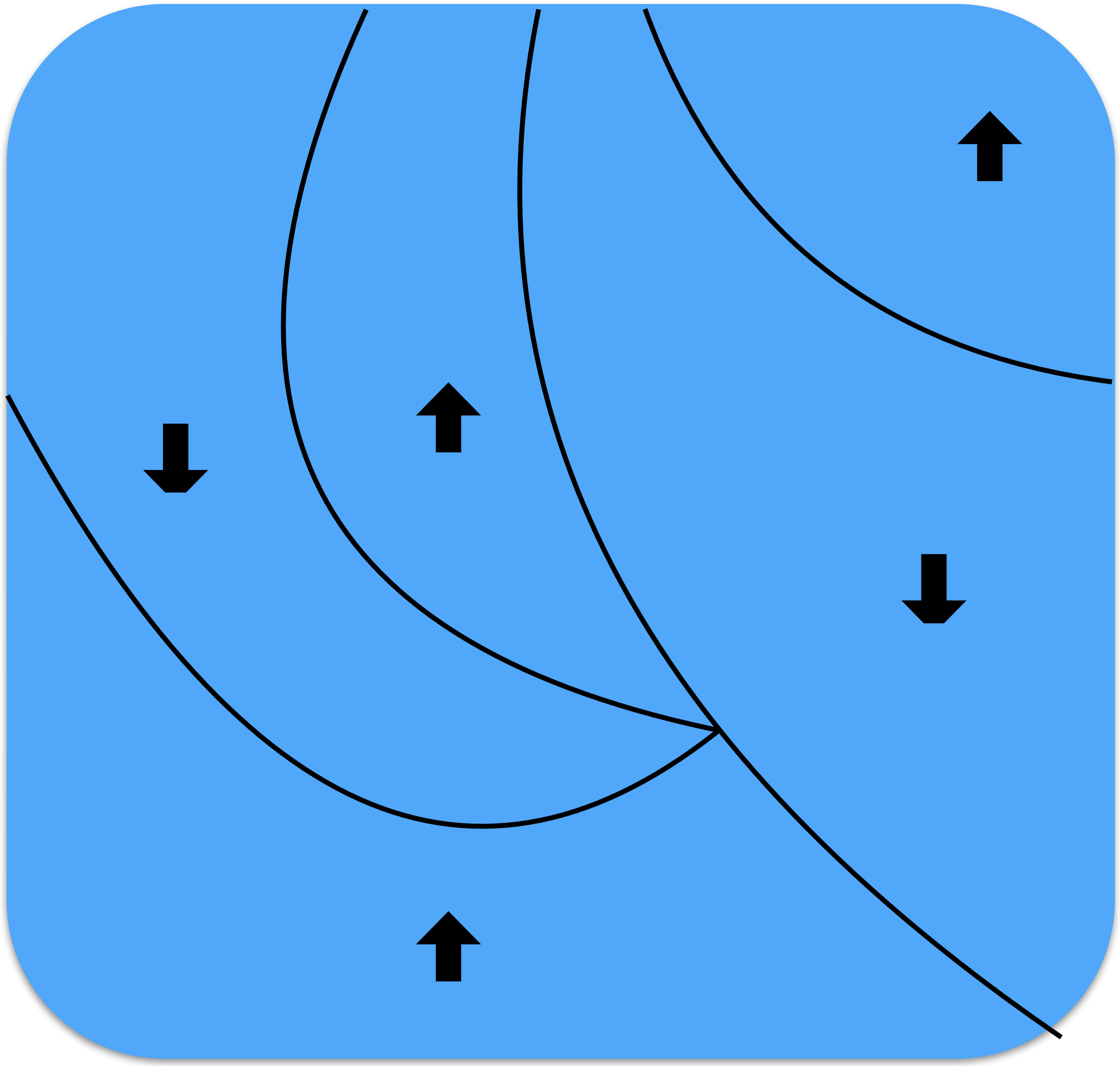
[see Poster P.03 “Random walks in Random Environments” by M.-A. García-March]

Model the membrane as an Ising lattice: $H = -J \sum_i \sigma_i \sigma_{i+1}$ $\sigma_i = \uparrow, \downarrow$

Link diffusivity to local membrane state

(e.g. faster diffusion on $\uparrow$ background)

Allow walker to locally modify
the membrane state



Kinetic Ising Model for the membrane

- Kinetic Ising Model: $\dot{P}(\sigma,t) = \sum_{\sigma'}[w(\sigma' \to \sigma)P(\sigma',t) - w(\sigma \to \sigma')P(\sigma,t)]$

  w: transition rate

- Interacting membrane: $w(\sigma_i \to -\sigma_i) = \frac{\alpha}{2}\left[1 - \frac{\gamma}{2}\sigma_i(\sigma_{i-1}+\sigma_{i+1})\right]$

  α/2: single spin-flip rate
  γ>0: IFM
  γ<0: AFM

- Detailed balance at equilibrium: $P_{\mathrm{eq}}(\sigma_1,\ldots,\sigma_i,\ldots,\sigma_n)w(\sigma_i \to -\sigma_i) = P_{\mathrm{eq}}(\sigma_1,\ldots,-\sigma_i,\ldots,\sigma_n)w(-\sigma_i \to \sigma_i)$

- $P_{\mathrm{eq}}(\sigma_1,\ldots,\sigma_i,\ldots,\sigma_n) \propto \exp[\beta J \sigma_i(\sigma_{i-1}+\sigma_{i+1})]$

  $q_i(t) = \langle \sigma_i(t) \rangle$
  $r_{i,k}(t) = \langle \sigma_i(t)\sigma_k(t) \rangle$

- $P(\sigma,t) = \frac{1}{2^N}\sum_{\{\sigma'\}}(1+\sigma_1\sigma_1')\ldots(1+\sigma_N\sigma_N')P(\sigma',t) = \frac{1}{2^N}\left\{1 + \sum_i \sigma_i q_i(t) + \sum_{i\neq k}\sigma_i\sigma_k r_{i,k}(t) + \ldots\right\}$

- Recursive system of differential equations: e.g., $\alpha^{-1}\dot{q}_i(t) = -q_i(t) + \gamma/2[q_{i-1}(t) + q_{i+1}(t)]$

- **Exact time-dependent solutions** may be found for: infinite lattice, single spin fixed, (time-delayed) spin correlations, spin systems in a magnetic field, …

R. Glauber, *Time-dependent statistics of the Ising model*, J. Math. Phys. (1963)

Kinetic Ising Model for membrane+walker

- Master equation: $\dot{P}(\sigma, x, t) = [\gamma_s \mathcal{L}_s + \gamma_w \mathcal{L}_w] P(\sigma, x, t)$

s: spins (=membrane)
w: walker
x: position of the walker

- The walker may act as a localized potential for the spins, or it may change the tunneling between the neighboring spins

- If either the spins or the walker dynamics is fast, we may use an adiabatic approximation

- E.g., $\gamma_s \gg \gamma_w \quad \rightarrow \quad \mathcal{L} = \gamma_s \left[\mathcal{L}_s + \frac{\gamma_w}{\gamma_s} \mathcal{L}_w \right]$ and $P(\sigma, x, t) \sim P_w(x, t|\sigma) P_s^{(\mathrm{eq})}(\sigma|x)$
    - polaronic behavior (rapid formation of a dressing cloud, dragged along by the walker)

- In the opposite limit instead, the walker spreads very fast, and will act as a diffuse potential (mean-field) for the membrane

(Quantum) Kinetic Ising Models

- Ansatz: $P(\sigma, t) = \sqrt{P_{\mathrm{eq}}(\sigma)}\phi(\sigma, t)$

- The KIM master equation may be written as $\dot{\phi}(\sigma, t) = -\sum_{\sigma'} H_{\sigma\sigma'}\phi(\sigma', t)$

$$H_{\sigma\sigma'} = \sum_{\sigma''} w(\sigma \to \sigma'')\delta_{\sigma\sigma'} - w(\sigma' \to \sigma)\sqrt{\frac{P_{\mathrm{eq}}(\sigma')}{P_{\mathrm{eq}}(\sigma)}}$$

- If the KIM satisfies a detailed-balanced condition, then H is a (real) symmetric matrix, so that the KIM-ME may be seen as a Schrödinger equation in imaginary time, which converges exponentially to the thermal equilibrium solution. Diagonalization of H is then equivalent to the complete solution of the KIM-ME

- Classical spins may be promoted to non-commuting Pauli matrices to obtain quantum models

- Quantum states built from thermal states of classical Hamiltonians, e.g., $|\Psi\rangle = \frac{1}{\sqrt{Z_N}}\sum_{\sigma} e^{-\beta H(\sigma)/2}|\sigma\rangle$ *fulfill the area law in any dimension, even at criticality*, and can be represented efficiently as matrix product states (MPS), or projected entangled pair states (PEPS)

Augusiak, Cucchietti, Haake & Lewenstein, New J. Phys. (2010)

Quantum Brownian Motion

- A small system interacting with a large thermal bath: $H = H_S + H_B + H_I$

- Simplest interaction: $H_I = -\sum_k \kappa_k x_k x$

x_k: position of the k[th] oscillator
κ_k: coupling constant
x: position of the system

- ME for the reduced density matrix: $\dot{\rho}_S(t) = -\frac{1}{\hbar^2}\int_0^t \mathrm{d}s \, \mathrm{Tr}_B[H_\mathrm{I}(t), [H_\mathrm{I}(s), \rho(s)]]$

- Born approx.: $\rho(t) \simeq \rho_S(t) \otimes \rho_B(0)$

- Markov approx.: the bath evolves on timescales much faster than the system, and as such effectively retains no memory of the system's dynamics

- The spectral density contains all details of the bath-system coupling: $J(\omega) \equiv \sum_k \frac{\kappa_k^2}{2m_k\omega_k}\delta(\omega - \omega_k)$

Born-Markov QME

- Weak-coupling limit (second-order perturbation in H_I)

- Ohmic spectral density with Lorentz-Drude cut-off: $J(\omega) = \frac{m\gamma\omega}{\pi}\frac{\Lambda^2}{\omega^2 + \Lambda^2}$

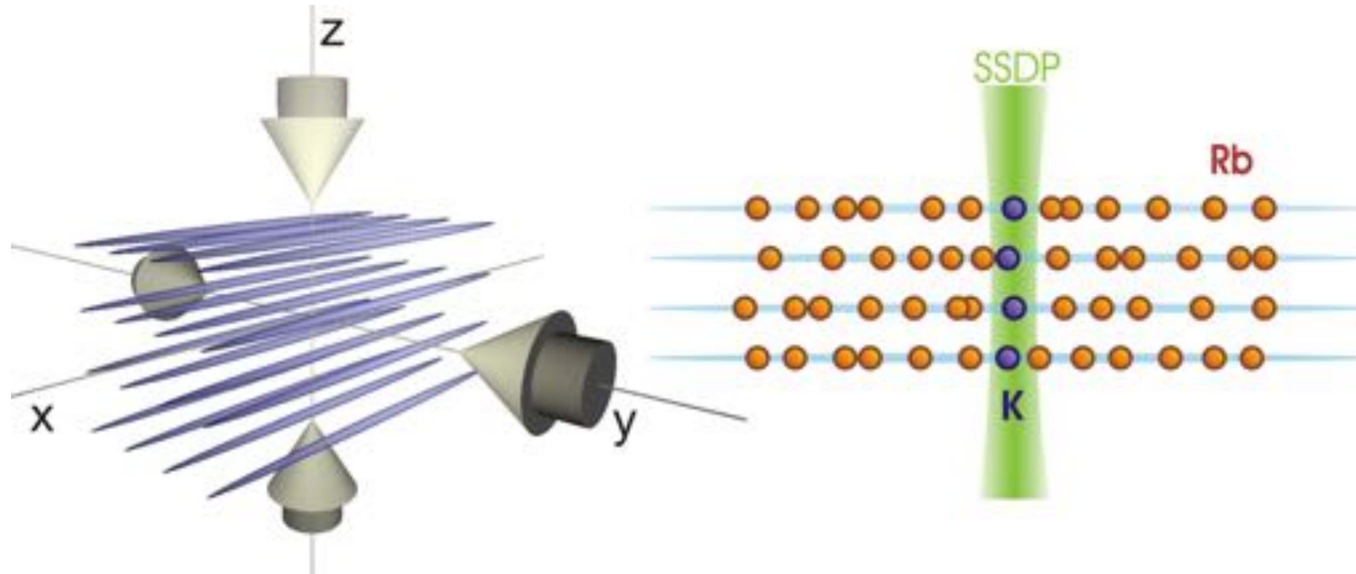
- Consider a particle of mass m in a harmonic trap of frequency Ω. In the high-temperature limit $k_B T \gg \hbar\Lambda \gg \hbar\Omega$ one obtains the celebrated Caldeira-Leggett QME:

$$\dot{\rho}_S = -\frac{i}{\hbar}[H_{\rm sys}, \rho_S] - \underbrace{\frac{i\gamma}{2\hbar}[x, \{p, \rho_S\}]}_{\text{momentum damping}} - \underbrace{\frac{m\gamma k_B T}{\hbar^2}[x, [x, \rho_S]]}_{\text{normal diffusion}}$$

- A quantum stochastic process is said to be Markovian only if the underlying noise is white, and if the process is described by a time-independent ME of the Lindblad form

- Note that there exists an *exact* solution of the QBM problem, which however has a time-dependent Liouvillian. Strictly-speaking, QBM is not a quantum Markov process.

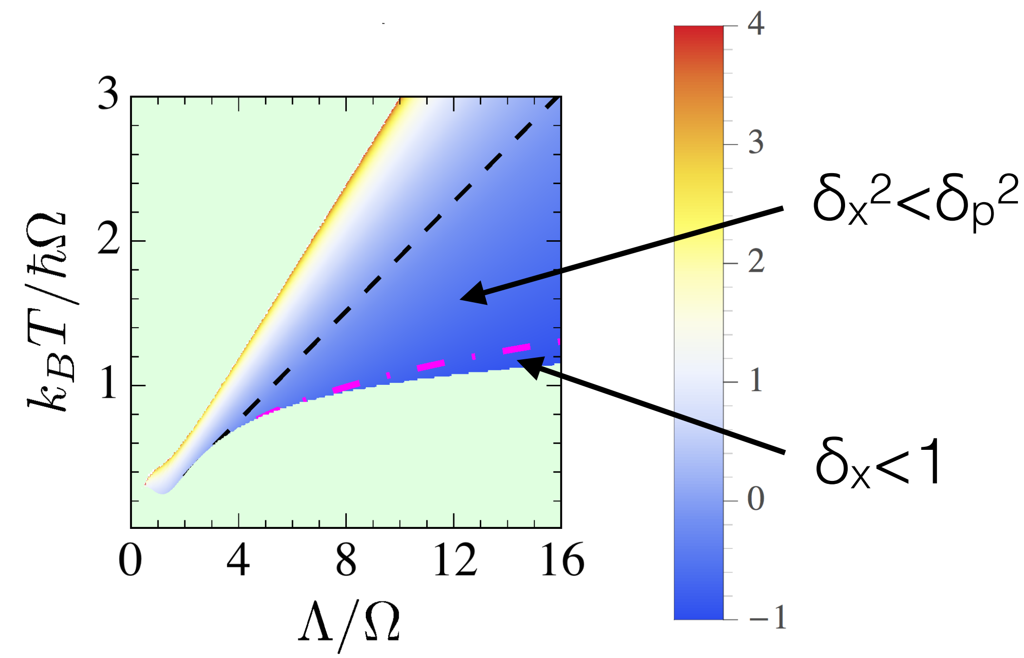
Impurities in an inhomogeneous 1D BEC



Catani et al., Phys. Rev. A (2012)

How to treat a spatially-dependent profile of the bath?
Coupling which is a non-linear function of the system's position: $H_I = -\sum_k \kappa_k x_k f(x)$

Aspect ratio of the impurity, $\ln(\delta_p^2/\delta_x^2)$,
for a quadratic coupling with the environment:



How to deal with the low temperatures of a quantum gas?
Non-Markovian effects will become important here!

And what if the spectral density is not Ohmic?
(i.e., the noise is not white)

PM, Lampo, Wehr & Lewenstein, Phys. Rev. A (2015)

Open questions

A. Classical

- Anomalous diffusion in biological systems

Q: mechanisms leading to sub- or super-diffusion, Levy flights, non-stationarity and non-ergodicity?

- Kinetic Ising Models

Q: mechanisms generating interactions between walkers and substrates?

B. Quantum

- Quantum Kinetic Ising Models

Q: novel exactly or efficiently solvable quantum Hamiltonians?

- Quantum Brownian Motion

Q: importance of non-Markovian effects at low temperatures?

Conclusions

- Walkers on largely heterogeneous substrate can exhibit strongly subdiffusive and non-ergodic behavior, even without transient immobilization

  PM, Manzo, Torreno-Pina, García-Parajo, Lewenstein & Lapeyre, Phys. Rev. Lett. (2014)
  Manzo, Torreno-Pina, PM, Lapeyre, Lewenstein & García-Parajo, Phys. Rev. X (2015)

- We are working towards describing membrane-walkers interactions by means of Kinetic Ising Models (KIMs)

- KIMs may be generalized to the quantum domain

- Quantum Brownian Motion in presence of an inhomogeneous background may be described by couplings which are polynomial functions of the system variables

  PM, Lampo, Wehr & Lewenstein, Phys. Rev. A (2015)

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THANK YOU!