# Quasi-two-dimensional dispersion dynamics of protein monolayers

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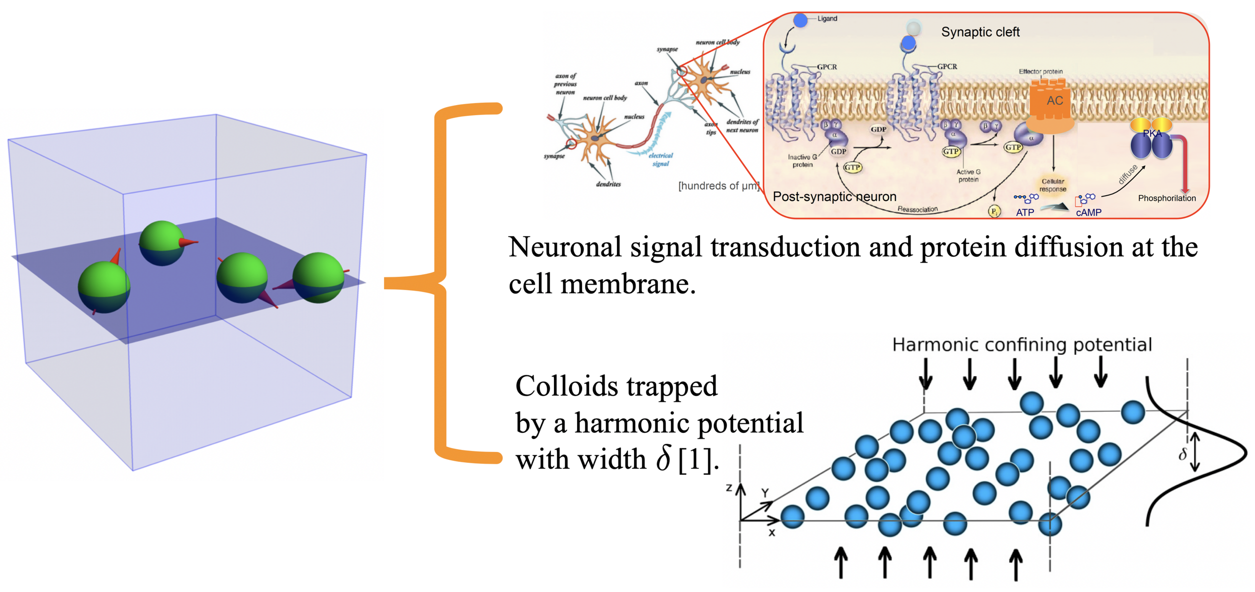
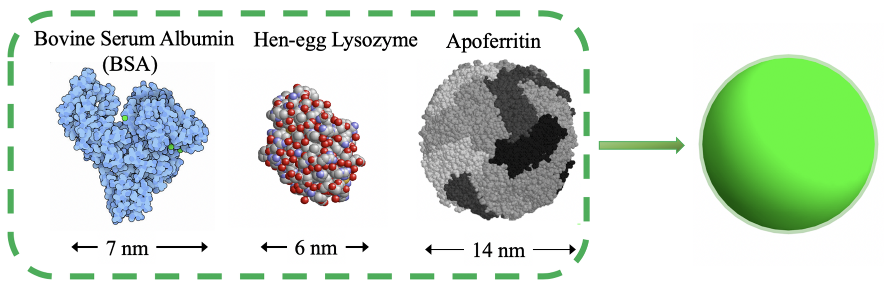
## 1. Motivation

- Interacting Brownian particles embedded in a three-dimensional (3D) bulk fluid but confined to a planar monolayer are frequently encountered in (biological) soft matter systems: (a) Proteins laterally diffusing along a cell membrane such as in postsynaptic neuronal signal transduction involving G-alpha proteins; (b) Colloids trapped at a fluid-fluid interface and interacting via electrostatic and surface capillary forces [1].
- The interplay of in-plane translational particle motions and solvent-mediated 3D fluid dynamics gives rise to peculiar effects such as enhanced large scale collective diffusion [2].
- Using mesoscale simulations, we explore the effects of hydrodynamic and direct interactions on the dynamics of globular protein monolayers at different time scales.

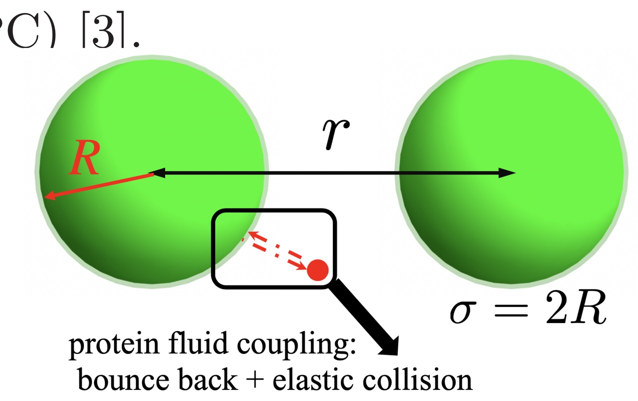



## 2. Numerical model




Globular proteins $\Longrightarrow$ Sphere

- Effective sphere model mimics globular proteins. Out-of-plane fluid motion is described by multiparticle collision dynamics (MPC) [3].



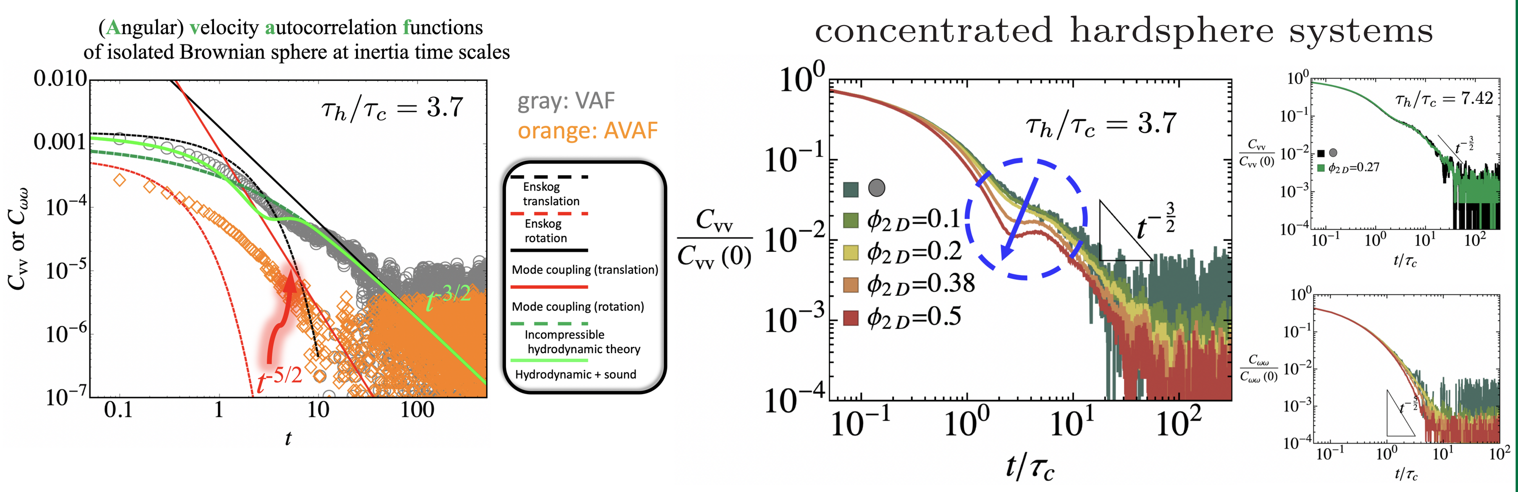

- Proteins interact via short-range attraction (SA) and long-range electrostatic repulsion (LR) [4]. The direct pair potential is given by

$$\beta U(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{100} - \left(\frac{\sigma}{r}\right)^{50}\right] + \ell_B Z_{eff}^2 \frac{e^{-r/\lambda}}{r}$$

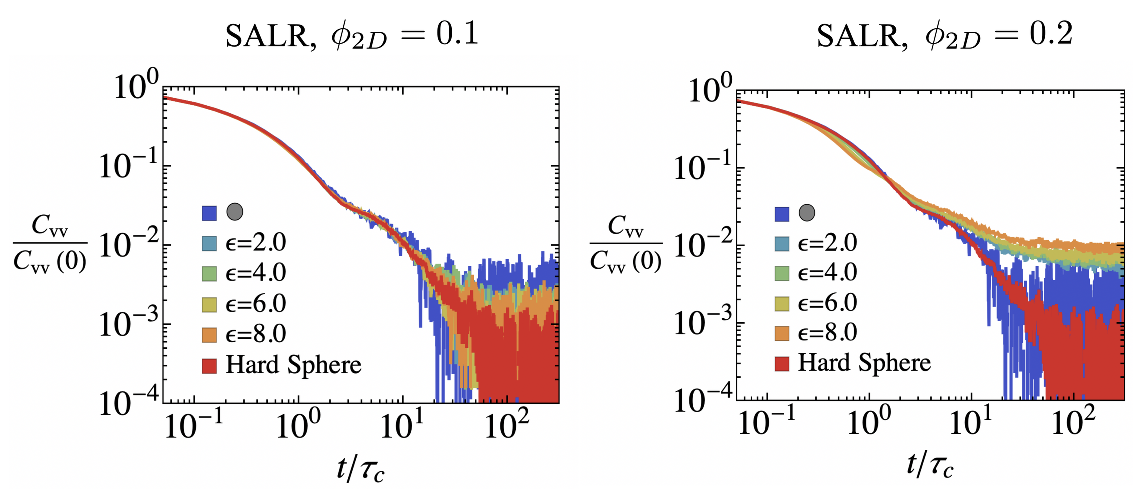
hardcore + short-range attraction | long-range repulsion

## 4. Q2D Brownian motion on inertial time scales

- **Hydrodynamic retardation**
  - sound propagation (time $\tau_c = R/c$)
  - shear wave diffusion ($\tau_h = R^2\rho_f/\eta$)
- Sound induced back-tracking presents in translational dynamics for $\tau_h < \tau_c$ only (left figure). Long-time tails are visible in (angular) colloidal velocity autocorrelation functions (VCF: $C_{vv}$; AVCF: $C_{\omega\omega}$).




- In concentrated hard sphere systems (upper-right figures), albeit $\tau_h > \tau_c$, back-tracking reappears. Increasing $\phi_{2D}$ results in shorter inter-particle distances and enhances multiple sound waves scattering.
- Long-time power-law decay of translational VAF also in concentrated systems.

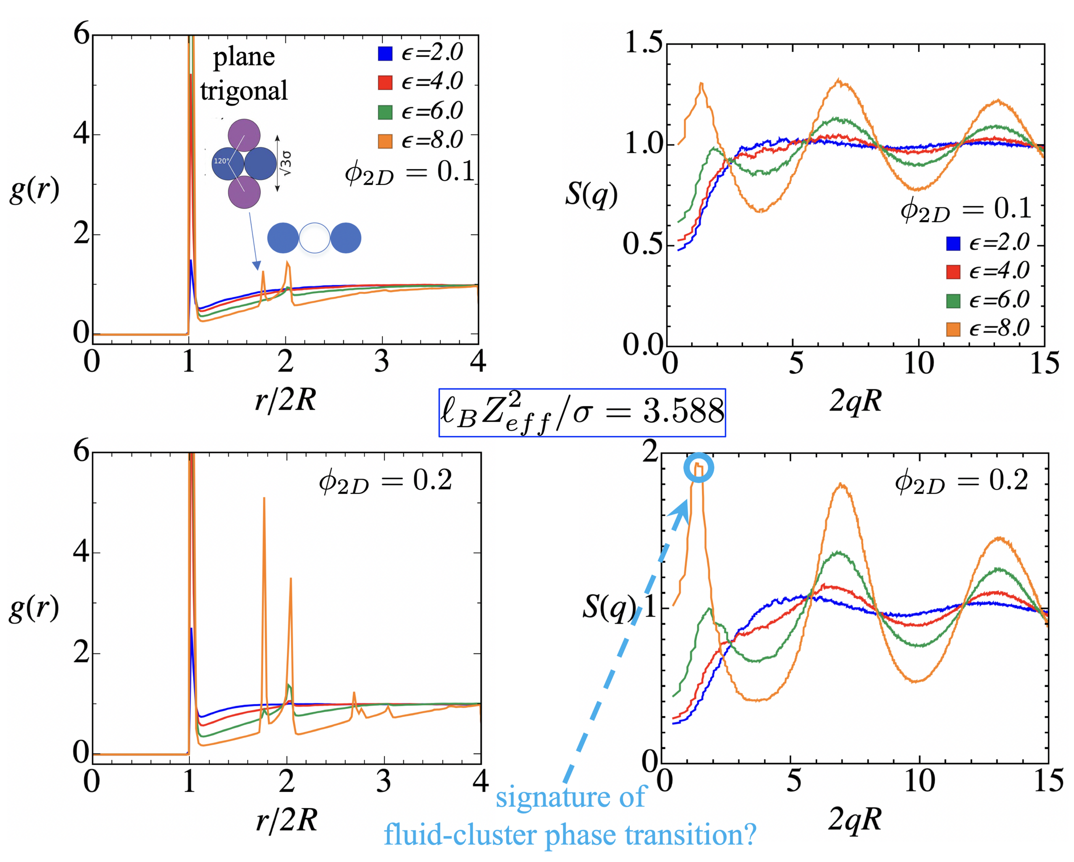



- Our preliminary results suggest that direct interactions in SALR systems are of importance also at inertial time scales. Attraction slows particle dynamics.

## 3. Structure of Q2D-SALR systems

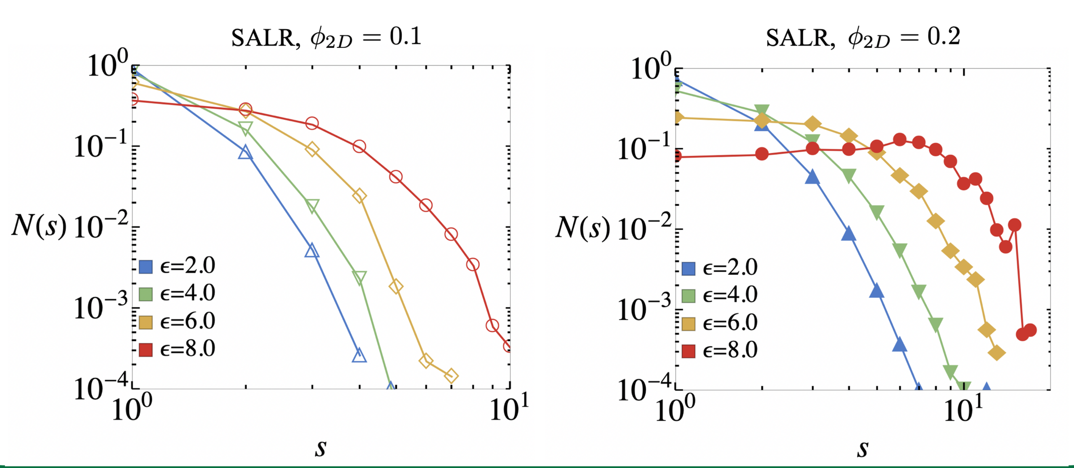
We first identify dispersed-fluid phase systems whose dynamics we explore subsequently.

- Radial distribution function $g(r)$ and static structure factor $S(q)$




- Cluster size distribution function $N(s)$:

$$N(s) = \left\langle \frac{s}{N_p} n(s) \right\rangle \qquad \sum_{s=1}^{N_p} N(s) = 1$$

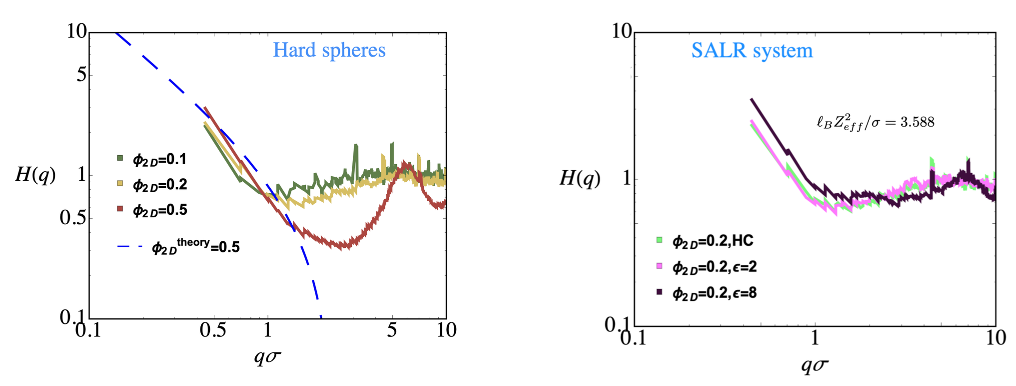



## 5. Short time collective diffusion

The collective diffusion function $D_c(q)$ of proteins characterizes the short-time relaxation ($\tau_h \ll t \ll R^2/D_0$) of sinusoidal density fluctuations of wavenumber $q$. Experimentally, it can be deduced from the dynamic structure factor S(q,t) for isotropic systems:

$$\frac{S(q,t)}{S(q)} = \exp\left[-q^2 D_c(q) t\right] = \exp\left[-\frac{D_0 H(q)}{S(q)} q^2 t\right]$$

- **Hydrodynamic function** $H(q)$ includes full information on short-time diffusion:




Long wavelength approximation [4]:

$$H(q < 1/\sigma) \approx 1 + \frac{3\phi_{2D}}{q\sigma} + \frac{9\phi_{2D}}{2\sigma}\int_0^\infty dr[g(r) - 1]$$

- H(q) diverges like $1/(qL_h)$ for $q << 1/L_h$
- Hydrodynamic length $L_h = \sigma/(3\phi_{2D})$
- Interactions alter overall magnitude of $H(q)$ but leave $1/q$ divergence in Q2D systems unaffected.

**Why?**

1. Fully developed 3D hydrodynamics gives rise to apparent in-plane fluid compressibility and long-range particle correlations. [2].
2. Transversal transport of fluid momentum induces effective inter-particle repulsion [6].

## 6. Work in progress

1. Sound propagation in concentrated Q2D systems: wavenumber dependent (distinct) current-current correlation function.
2. Influence of direct interactions and concentration changes on long-wavelength hydrodynamic enhancement.
3. Generalized time-dependent hydrodynamic function $H(q,t)$.
4. Intermediate-time and long-time collective and self-diffusion properties.
5. Effect of anisotropic interactions e.g., dipolar potential.
6. Protein diffusion dynamics at liquid-liquid interface.

## 7. References

[1] S. Panzuela, R. P. Peláez, and R. Delgado-Buscalioni, *Phys. Rev. E*, **95**, 012602 (2017).

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