Quasi-two-dimensional dispersion dynamics of protein monolayers

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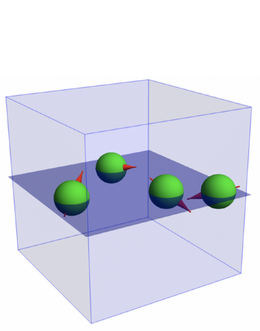
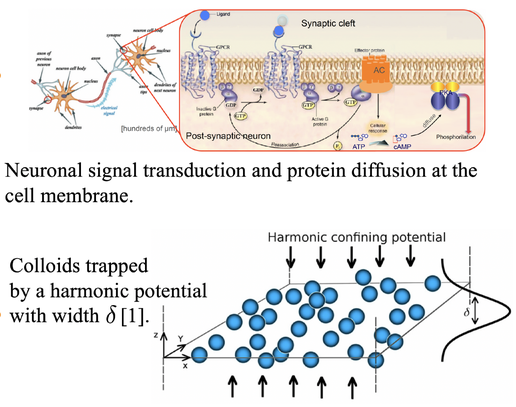
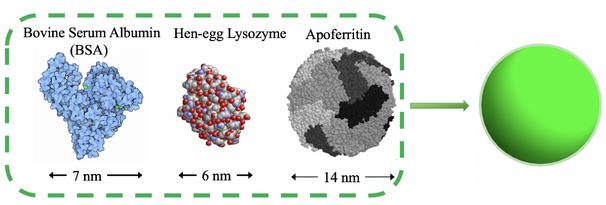
1. Motivation

- ◇ 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.



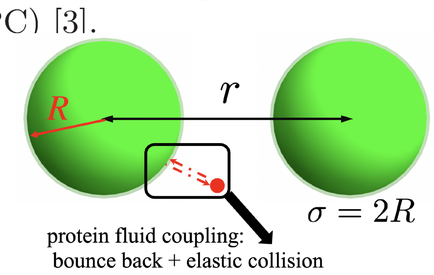


2. Numerical model



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

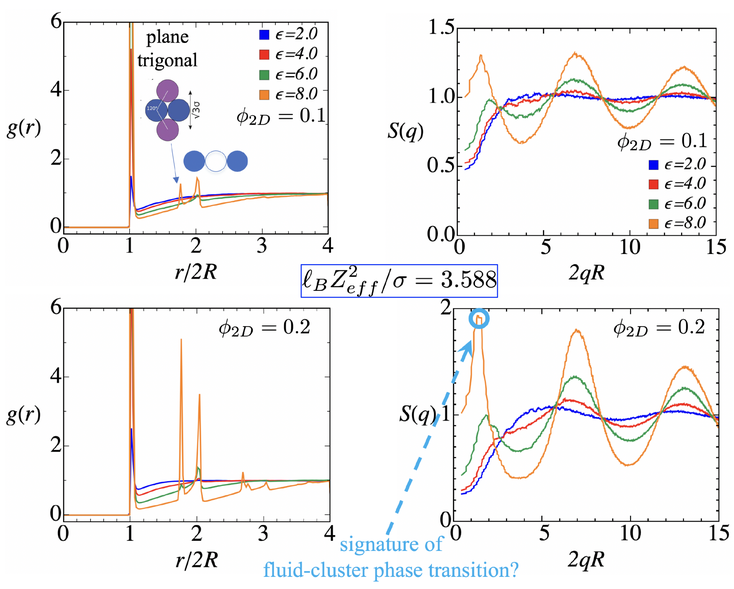
$$\beta U(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{100} - \left(\frac{\sigma}{r}\right)^{50}\right] + \ell_B Z_{eff}^2 \frac{e^{-r/\lambda}}{r}$$

hardcore + short-range attraction — long-range repulsion

3. Structure of Q2D-SALR systems

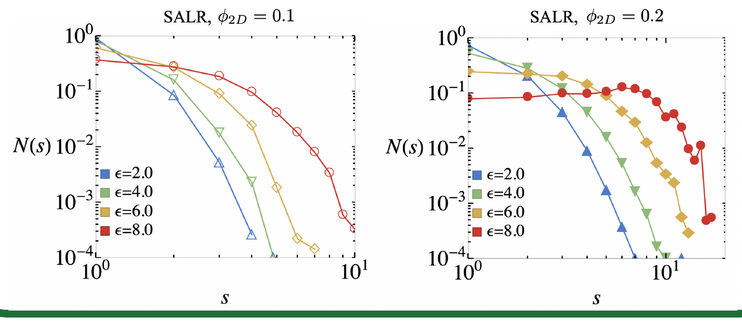
We first identify dispersed-fluid phase systems whose dynamics we explore subsequently.

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



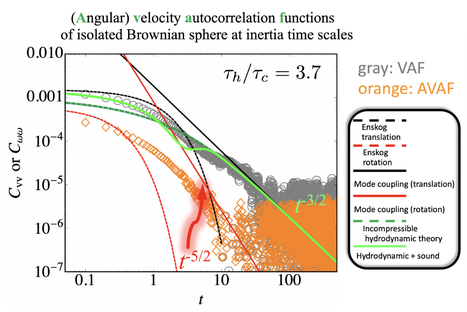
- ◇ Cluster size distribution function $N(s)$:

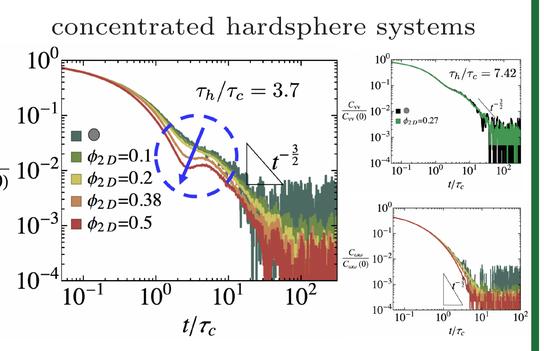
$$N(s) = \left\langle \frac{s}{N_p} n(s) \right\rangle \qquad \sum_{s=1}^{N_p} N(s) = 1$$



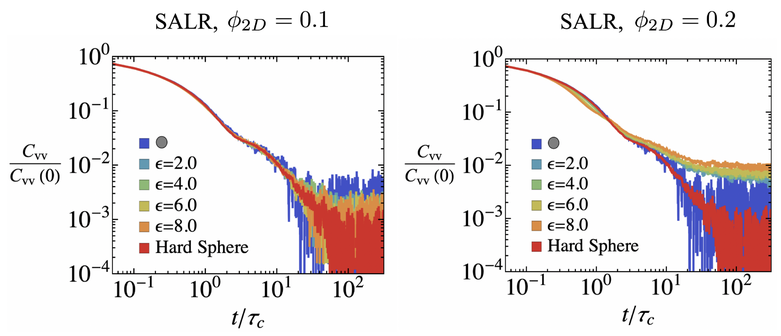
4. Q2D Brownian motion on inertial time scales

- ◇ **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: $C_{\omega\omega}$).





- Long-time power-law decay of translational VAF also in concentrated systems.



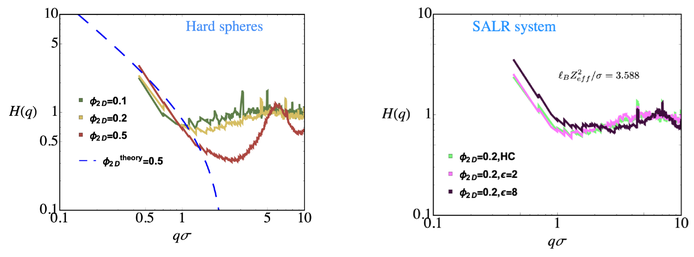
- Our preliminary results suggest that direct interactions in SALR systems are of importance also at inertial time scales. Attraction slows particle dynamics.

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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[3] G. Gompper, T. Ihle, D. M. Kroll, and R. G. Winkler, *Adv. Polym. Sci.*, **221** 1 (2009)

[4] S. Das, J. Riest, R. G. Winkler, G. Gompper, J. K. G. Dhont, and G. Nägele, *Soft Matter*, **14**, 92-103 (2018).

[5] M. Belushkin, R. G. Winkler, and G. Foffi, *J. Phys. Chem. B*, **120**, 14263–14268 (2011).

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