Models and effects of spatially correlated noise in stochastic dynamics

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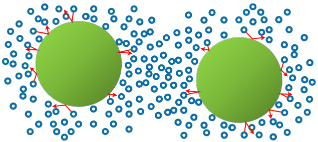
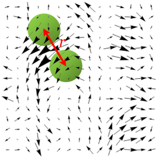
Spatio-temporal correlations in stochastic dynamics



subsystem coupled to another system

$\Rightarrow$



subsystem + noise + dissipation

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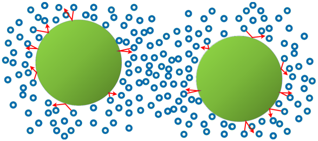

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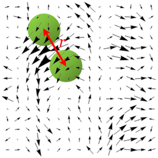

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- Langevin eq.: $m\ddot{x} + \gamma\dot{x} = F(x) + \sigma\eta(t)$, $< \eta(t)\eta(t') > \propto \delta(t-t')$, $\frac{\beta\sigma^2}{2} = \gamma$

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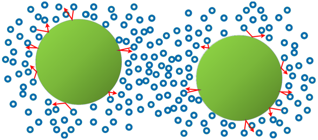

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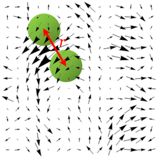

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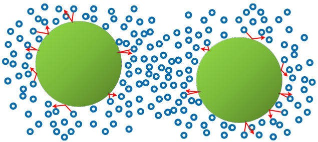

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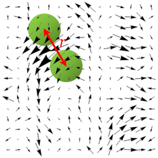

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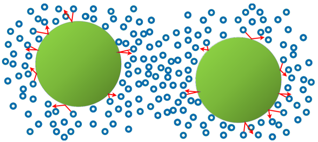

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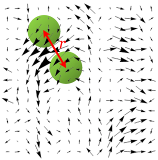

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spatio-temporal
correlations
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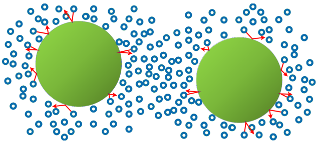

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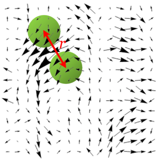

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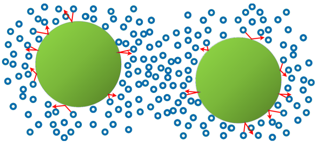
$\Downarrow$

theory?

Spatio-temporal correlations in stochastic dynamics



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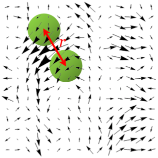

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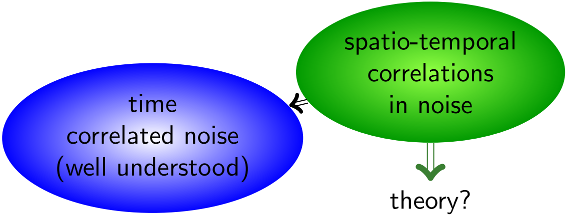

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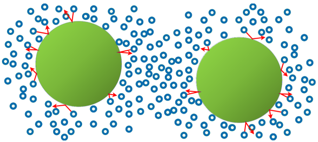

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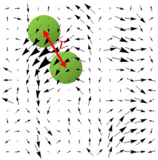

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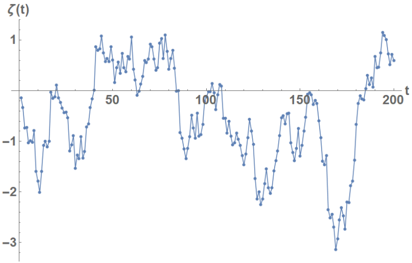
spatio-temporal correlations in noise

time correlated noise (well understood) $\Leftarrow$ $\Rightarrow$ spatially correlated noise (...not so well)

$\Downarrow$

theory?

Dynamics with time correlated noise



- **single** signal, $\zeta(t)$ and $\zeta(t')$ are related

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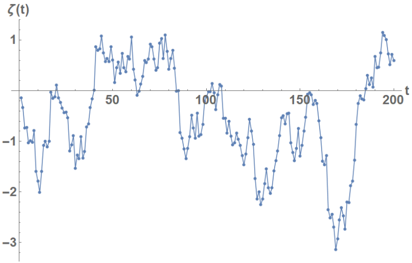


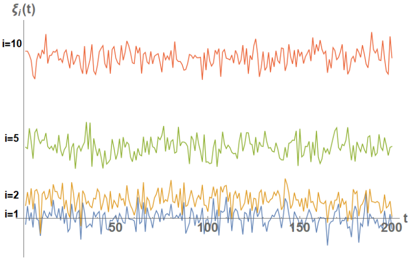
- **single** signal, $\zeta(t)$ and $\zeta(t')$ are related
- Generalized Langevin Equations:

$$\int_{-\infty}^{t} dt' \Gamma(t-t')\dot{x}(t') = F(x) + \zeta(t), \quad <\zeta(t)\zeta(t')> \propto \Gamma(t-t')$$

- $\Gamma(t-t')$ - memory kernel

Dynamics with spatially correlated noise (**SCN**)

- **multiple** signals
- $\xi_i(t)$ is realted to $\xi_j(t)$ ...
- ...but $\xi_i(t)$ independent of $\xi_i(t')$



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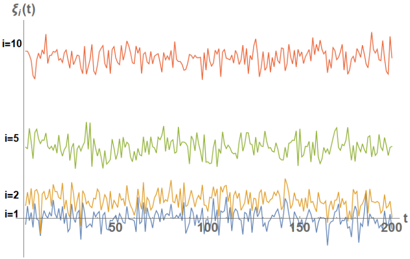


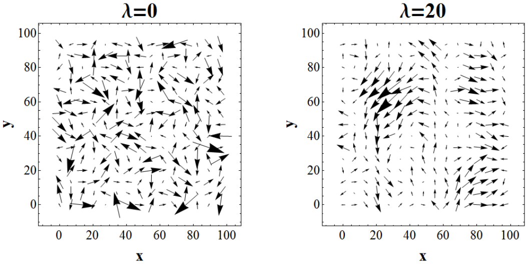
Langevin dynamics with SCN

$$\sum_j \Gamma(x_i - x_j)\dot{x}_j = \sum_j F(x_i - x_j) + \xi_i(t)$$

$$< \xi_i(t)\xi_j(t') > \propto h(x_i - x_j)\delta(t - t')$$

$\Gamma(x_i - x_j)$ - **collective dissipation**

- non-correlated noise vs. SCN on a grid:



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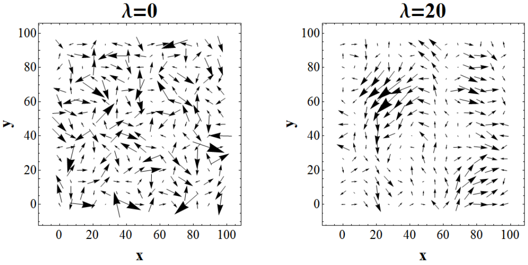
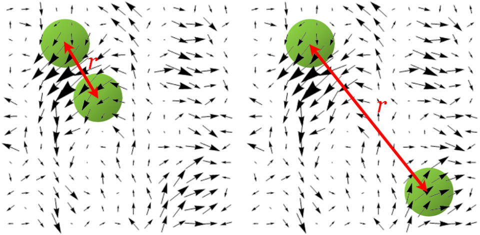


- Nearby vs. distant probes:

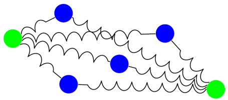


Models of SCN

Mori-Zwanzig microscopic model

q_n - $\tilde{N}$ heath-bath particles (oscillators), x_i - N observed tracers

$$M\ddot{x}_i = \sum_j^N F(x_i - x_j) + \sum_n^{\tilde{N}} c_{in}\left(q_n - \frac{2c_{in}}{mw_{in}^2}x_i\right)$$



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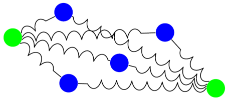

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Solve for $q(t) \Rightarrow$ effective dyn. of $x_i(t)$:

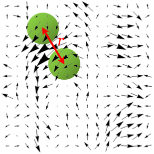
$$M\ddot{x}_i = \sum_j^N [F(x_i - x_j) + F_{eff}] - \sum_j^N \int_{t_0}^t dt'\Gamma_{ij}(t-t')\dot{x}_j(t') + \xi_i(t)$$

$$\Gamma_{ij}(t-t') = \sum_n^{\tilde{N}} \frac{c_{in}c_{jn}}{m\omega_n^2}\cos\omega(t-t') =< \xi_i(t)\xi_j(t') >$$

M. Majka, P. F. Góra, J. Phys. A: Math. Theor., 50, 5, 054004 (2017)

SCN-driven 2-particle dynamics

- Over-damped eq. of motion, $F(r) = -\partial_r U(r)$ and γ is const:



$$\gamma \dot{x}_1 = F(x_1 - x_2) + \xi_1$$
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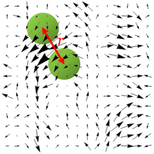

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- Change of variables: $R = (x_1 + x_2)/2$ and $r = (x_2 - x_1)/2$:

$$\gamma \dot{r} = 2F(r) + \xi_2 - \xi_1 \;\; \gamma \dot{R} = \frac{1}{2}(\xi_2 + \xi_1)$$

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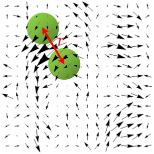

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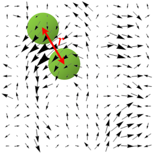

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Noise recombination

replace correlated noise with multiplicative non-correlated noise

$$\xi_2 \pm \xi_1 = \sqrt{2}\sigma\sqrt{1 \pm h(r)}\eta_\pm = \sqrt{2}\sigma g_\pm(r)\eta_\pm(t)$$

where $\eta_\pm$ comes from the normal distribution and:

$$< \eta_+(t)\eta_-(t') >= 0 \qquad < \eta_+(t)\eta_+(t') >=< \eta_-(t)\eta_-(t') >= \delta(t - t')$$

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- (x_1, x_2) dyn. with SCN $\Rightarrow$ (R, r) dyn. with multiplicative noise:

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- corresponding Fokker-Planck Equation (FPE):

$$\partial_t P = -\partial_r\left(\frac{2F(r)}{\gamma}P\right) + \sigma^2\partial_r\left[\frac{g_-(r)}{\gamma}\partial_r\left(\frac{g_-(r)}{\gamma}P\right)\right] + \frac{\sigma^2}{4}g_+^2(r)\partial_{RR}P$$

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- Stationary $\partial_t P = 0$ solution of FPE:

$$P(r, R) = \exp\left(\frac{2\gamma}{\sigma^2} \int_0^r dr' \, \frac{F(r')}{g_-^2(r')} - \ln \frac{g_-(r)}{\gamma} + C \right)$$

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Problem with SCN!

For $g_-(r) \neq 1$ this solution cannot be equal to Boltzmann distribution.

No thermodynamical consistency!

Spatially variant friction coefficient

Postulate:

Thermodynamical consistency for SCN requires friction coefficient that depends on the distance r

now, our equations of motion read:

$$\Gamma(r)\dot{r} = 2F(r) + \sqrt{2}\sigma g_-(r)\eta_-$$
$$\frac{\gamma}{2}\dot{R} = \frac{\sigma}{\sqrt{2}} g_+(r)\eta_+$$

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$$\Gamma(r)\dot{r} = 2F(r) + \sqrt{2}\sigma g_{-}(r)\eta_{-}$$
$$\frac{\gamma}{2}\dot{R} = \frac{\sigma}{\sqrt{2}} g_{+}(r)\eta_{+}$$

again, write down FPE, solve it:

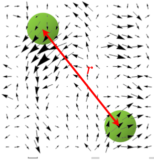
$$P(r,R) = \exp\left(\frac{2}{\sigma^2}\int_0^r dr' \frac{F(r')\Gamma(r')}{g_{-}^2(r')} - \ln\frac{g_{-}(r)}{\Gamma(r)} + C\right) = \exp(-\beta U(r))$$

$\Gamma(r)$ can compensate for $g_{-}(r) \Rightarrow$ we can restore Boltzmann dist.

SCN-driven 2-particle dynamics - basic properties

$$\Gamma(r)\dot{r} = 2F(r) + \sqrt{2}\sigma g_-(r)\eta_- \qquad \frac{\gamma}{2}\dot{R} = \frac{\sigma}{\sqrt{2}}g_+(r)\eta_+$$

$$\Gamma(r) = \frac{g_-(r)e^{-\beta U(r)}}{\frac{1}{\gamma} - \frac{2}{\sigma^2}\int_r^{+\infty} dr' \frac{F(r')}{g_-(r')}e^{-\beta U(r')}}$$



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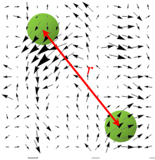
- classical relation $\gamma = \frac{\beta\sigma^2}{2}$ holds
- for non-correlated case $\Gamma(r) = \gamma$, as expected
- for huge r, $\Gamma(r) \to \gamma \Rightarrow$ ordinary Langevin dynamics



SCN-driven 2-particle dynamics - basic properties

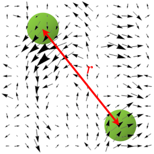
$$\Gamma(r)\dot{r} = 2F(r) + \sqrt{2}\sigma g_-(r)\eta_- \qquad \frac{\gamma}{2}\dot{R} = \frac{\sigma}{\sqrt{2}} g_+(r)\eta_+$$

$$\Gamma(r) = \frac{g_-(r)e^{-\beta U(r)}}{\frac{1}{\gamma} - \frac{2}{\sigma^2}\int_r^{+\infty} dr' \frac{F(r')}{g_-(r')} e^{-\beta U(r')}}$$

- classical relation $\gamma = \frac{\beta\sigma^2}{2}$ holds
- for non-correlated case $\Gamma(r) = \gamma$, as expected
- for huge r, $\Gamma(r) \to \gamma \Rightarrow$ ordinary Langevin dynamics
- $\Gamma(r) \Rightarrow$ **collective dissipation** in (x_1, x_2):

$$\frac{\gamma + \Gamma(r)}{2}\dot{x}_1 + \frac{\gamma - \Gamma(r)}{2}\dot{x}_2 = -F(r) + \xi_1$$

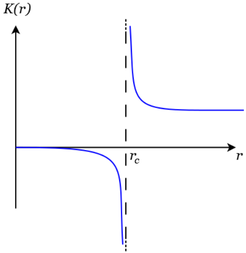
$$\frac{\gamma - \Gamma(r)}{2}\dot{x}_1 + \frac{\gamma + \Gamma(r)}{2}\dot{x}_2 = F(r) + \xi_2$$



$\Gamma(r)$ - singular behavior

$\Gamma(r)$ can become singular for certain critical $r = r_c$ satisfying:

$$\beta \int_{r_c}^{+\infty} dr' \frac{F(r')}{g_-(r')} e^{-\beta U(r')} = 1$$



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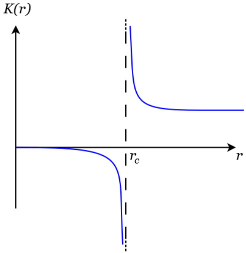
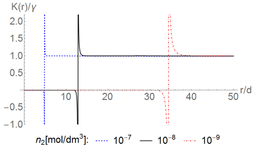


- a region of propulsion emerges
- linearized dynamics in the vicinity of r_c gives:

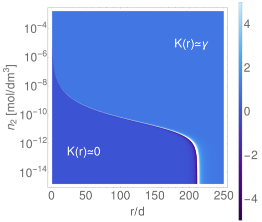
$$< r(t) >= r_c + (r_0 - r_c) \exp\left(\frac{4\beta F^2(r_c)}{\gamma g_-^2(r_c)} t\right)$$

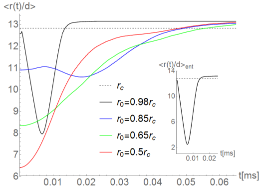
This result bifurcates, for $r_0 < r_c$ we get **decreasing** $< r(t) >$

2 surface-charged spheres and counter-ions

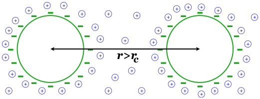


$\Gamma(r)$ for different concentrations n_2



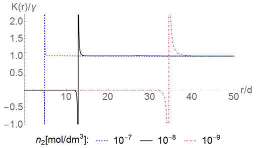


+inertia⇒transient attraction



$r > r_c$, each particle has its own layer of ions

2 surface-charged spheres and counter-ions



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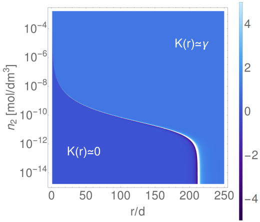

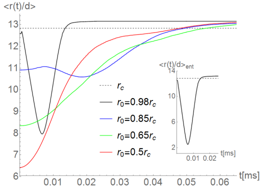

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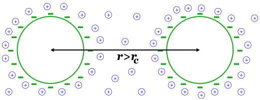

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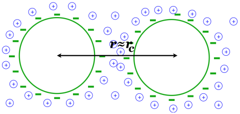
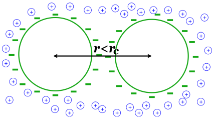
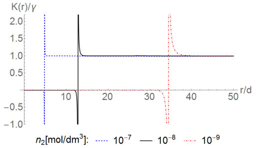


$r \simeq r_c$, layers 'feel' each other, peak in friction



$r < r_c$, layers reorganize into a single layer

2 surface-charged spheres and counter-ions



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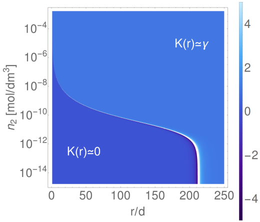

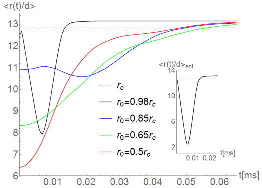

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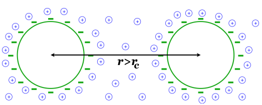

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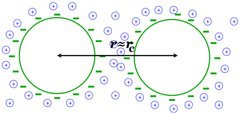

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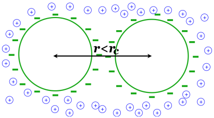


$r < r_c$, layers reorganize into a single layer

M. Majka, P.F. Góra, Phys. Rev. E, 94, 4, 042110 (2016)

Collective effects embedded in SCN!

Experimental confirmation?

Studies of transient effects are rare, but ⇒ E. Nagornyak, H. Yoo, and G. H. Pollack, Soft Matter 5, 3850 (2009)

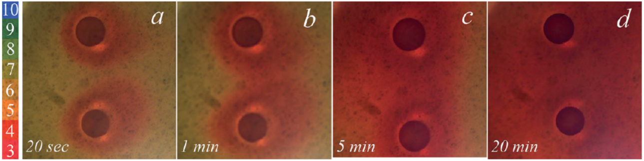
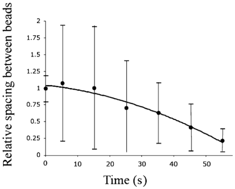


Fig. 3 Growth and propagation of low pH zone formed around negatively charged beads. pH scale shown in left panel.



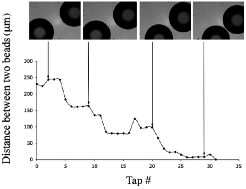


Fig. 1 Surface-to-surface distance between two beads following a series of taps, imparted every 2–3 seconds.

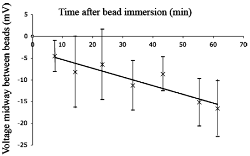


Fig. 5 Time dependence of electrical potential midway between beads. Standard deviations are shown as vertical lines. $n = 3$ experiments.

SCN-driven N-particle dynamics

- N particles in volume L, $\rho = N/L$, $F(r) = -\partial_r U(r)$, eq. of motion:

$$\sum_j^N \Gamma(x_i - x_j)\dot{x}_j = \sum_j^N F(x_i - x_j) + \xi_i$$

$$\mathbf{H}_{ij} = \sigma^2 h(x_i - x_j) = \rho \sum_k \hat{h}_k Q_{ik} Q_{jk} \quad \xi_i = \sum_k Q_{ik} \sqrt{\rho \hat{h}_k} \eta_k$$

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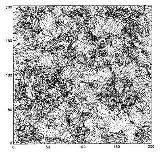
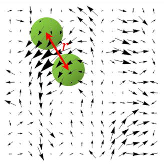
What are we looking for?

SCN-driven diffusion qualitatively resembles **dynamic heterogeneity**. Can SCN induce glass transition?



$\Longleftrightarrow$



SCN-driven N-particle dynamics

- Stationary FPE:

$$0 = \sum_i \partial_{x_i} \left([\mathbf{\Gamma}^{-1}\vec{F}]_i P_s \right) - \frac{1}{2} \sum_{i,j} \partial^2_{x_i x_j} \left([\mathbf{\Gamma}^{-1}\mathbf{H}\mathbf{\Gamma}^{-1}]_{ij} P_s \right)$$

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Solution in the limit $N \to +\infty, L \to +\infty$, $N/L = \rho$

$$\mathbf{\Gamma}_{ij} = \Gamma(x_i - x_j) = \frac{\gamma a_H}{\pi \rho} \int_0^{\frac{\pi m}{d}} dk \frac{\hat{h}(k)[2 + \beta\rho\hat{U}(k)] \cos k(x_i - x_j)}{1 + \hat{h}(k) + \beta\rho\hat{U}(k)}$$

M. Majka, P. F. Góra, https://arxiv.org/abs/1707.07076 (2017)

Glass-like transition in $\mathbf{\Gamma}_{ij}$

$$\mathbf{\Gamma}_{ii} = \frac{\gamma a_H}{\pi\rho} \int_0^{\frac{\pi m}{d}} dk \frac{\hat{h}(k)[2 + \beta\rho\hat{U}(k)]}{1 + \hat{h}(k) + \beta\rho\hat{U}(k)}$$

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$1 + \hat{h}(k) + \psi\hat{U}(k) = 0$ (**non-integrable** singularity) $\Rightarrow \mathbf{\Gamma}_{ii} \to +\infty$

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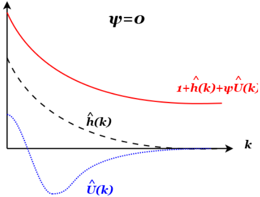

smooth $I(k,0)$

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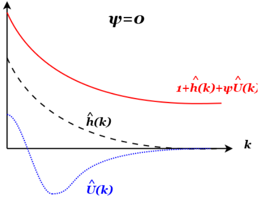

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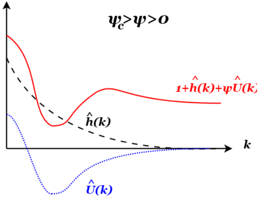

$I(k,\psi)$ develops a finite peak

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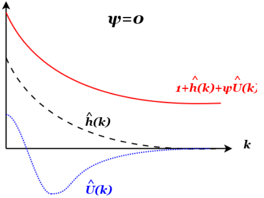

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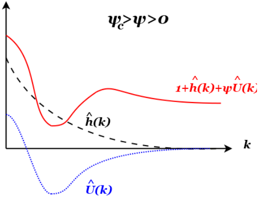

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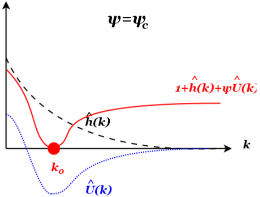
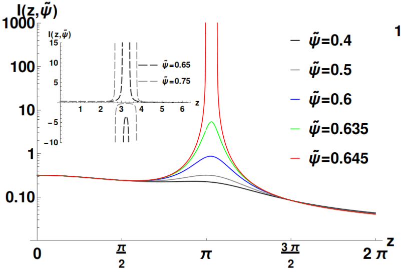
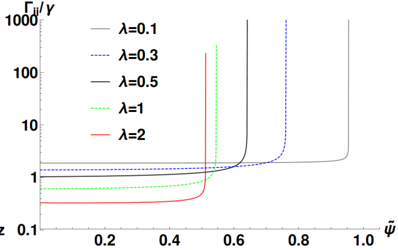


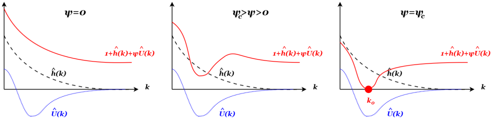
$I(k,\psi_c)$ has a non-integrable singularity

Glass-like transition in Γ_{ij} - divergence

correlations: $h(r) = e^{-r/\lambda}$, $\Gamma_{ii} \propto (\psi_c - \psi)^{-1/2}$

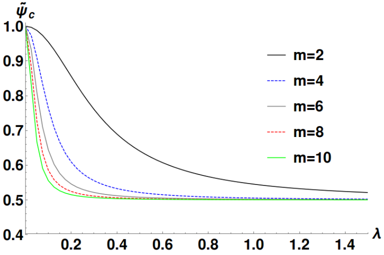






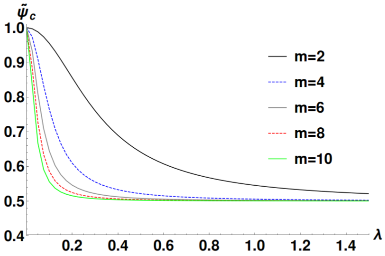
Glass-like transition in Γ_{ij}

- critical packing vs. corr. length



Glass-like transition in $\boldsymbol{\Gamma}_{ij}$

- critical packing vs. corr. length

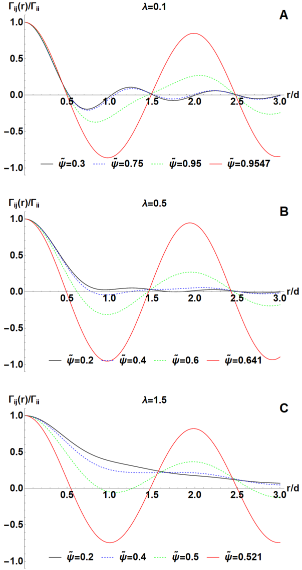


- Non-diagonal $\boldsymbol{\Gamma}_{ij}$ behaves as:

$$\frac{\boldsymbol{\Gamma}_{ij}}{\boldsymbol{\Gamma}_{ii}} \simeq e^{-\frac{r}{\theta_c}} \cos k_0 r$$

$$\theta_c \propto (\psi - \psi_c)^{-1/2}$$

θ_c - **collective dissipation length**



Langevin dynamics with SCN

$$\sum_j \Gamma(x_i - x_j)\dot{x}_j = \sum_j F(x_i - x_j) + \xi_i \quad < \xi_i \xi_j >= h(x_i - x_j)$$

SCN $\Rightarrow$ collective dissipation $\Rightarrow$ collective effects