Single-Particle Dynamics for Glassy Systems

recapitulation for collective dynamics:

- Mori-Zwanzig projections for variables $|\varrho_q\rangle$ and $|j^L_q\rangle$ → double fraction with density autocorrelation function and fluctuating force kernel → both become arrested at a putative glass transition
- second projection onto density pairs $|\varrho_k \varrho_p\rangle$ and factorization of four-point correlations into product of simple pairs yields closed equations
- long-time limit of normalized density autocorrelator $\phi_q(t) \xrightarrow{t\to\infty} f_q$ follows
  $$\frac{f_q}{1-f_q} = m_q[f_k]$$
  which exhibits glass-transition singularities for strong enough coupling
- expansion of MZ-eom around singularities results in scaling master functions and time divergences

How can single-particle variables be described?

exact representation after projection onto $|\rho^s_q\rangle$

$$\boxed{\hat{F}^s(q,z) = \frac{-1}{z + q^2 \hat{D}(q,z)}}$$

which is exact

To allow for a glass transition, diffusion coeff needs to go to zero exactly $D=0$, which is likely ruined if approximation is applied to $\hat{D}(q,z)$.

different approach: projection onto $|\rho^s_q\rangle$ and $|j^{sL}_q\rangle$ to allow for double fraction MZ representation even if $|j^s_q\rangle$ is not a conserved quantity

tagged particle correlator then follows $(\phi^s_q(t) = F^s(q,t))$

$$\boxed{\hat{\phi}^s_q(z) = \frac{-1}{z - \frac{\Omega^{s2}_q}{z + \Omega^{s2}_q \hat{m}^s_q(z)}}}$$

$$\Omega^{sL}_q = q^2 v_{th}^2$$

memory kernel $\hat{m}^s_q(z)$ at glass transition would be finite $\rightarrow$ approximation of $\hat{m}^s_q(z)$ more appropriate

choose second projector to couple to collective dynamics as

$$\boxed{P_2^s := |\rho_k^s \rho_p) \frac{1}{N S_p} (\rho_k^s \rho_p|}$$

yields tagged particle memory kernel

$$\boxed{m_q^s(t) = \sum_{k,p} V^s_{qkp}\, \phi_k^s(t)\, \phi_p(t)}$$

and the bifurcation equation for the tagged particle autocorrelator

$$\boxed{\frac{f_q^s}{1 - f_q^s} = m_q^s[f_k^s, f_p]} \quad (*)$$

and similarly for the MSD a memory kernel

$$\boxed{m^{(\omega)}(t) = \lim_{q \to 0} q^2 m_q^s(t)}$$

as well as a bifurcation equation

$$\boxed{\lim_{t \to \infty} \delta r^2(t)/6 = r_c^2 = 1/\lim_{t \to \infty} m^{(\omega)}(t)}$$

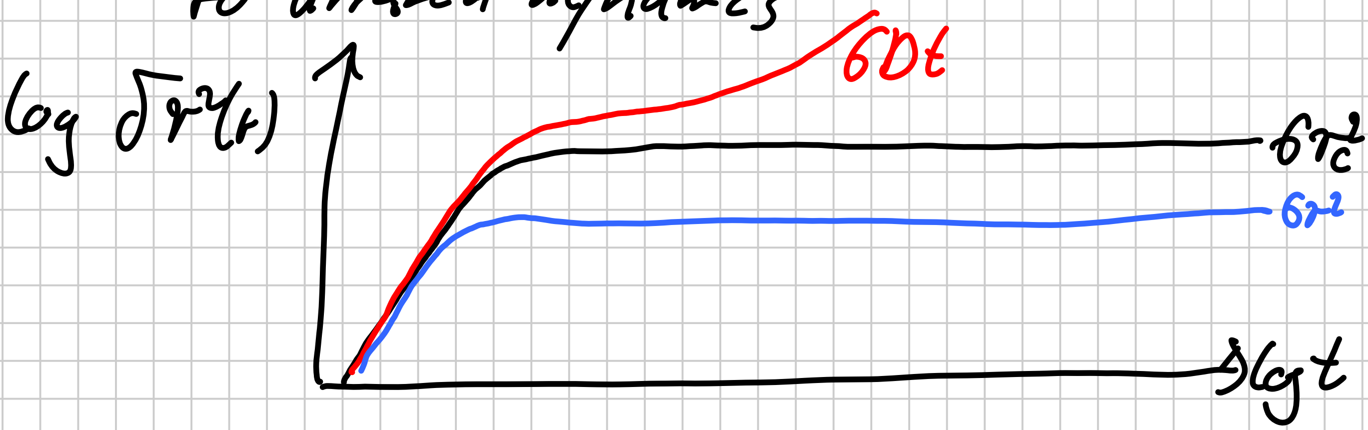
defining the localisation length r_c

remarks

1. bifurcations in (*) are inherited from the respective bifurcation in the collective dynamics for $\phi_q(t)$, identical asymptotic expansions for incoherent and coherent dynamics

(2) coupling of $\phi_q^s(t)$ to collective dynamics needs to be large enough to trigger arrest in f_q^s; for very small tagged particle $f_q^s = 0$ even for $f_q > 0$ since the V^s_{qkp} may be too small

(3) MSD at glass transition goes from diffusion to arrested dynamics



(4) mathematical mechanism for coupling a measurement variable (e.g. $\delta r^2(t)$) to the variable exhibiting the relevant bifurcation dynamics originally is generic: $\phi_q^s(t)$ may hence also describe light-scattering, neutron scattering, etc.