

Mode-Coupling Theory of the Glass Transition

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1 The basic framework of Mode-Coupling Theory (MCT)

The **Mode-Coupling Theory (MCT)** is the only known theory that are first-principles-based [1, 2]. It uses the Mori-Zwanzig formalism [3] to integrate out unnecessary degrees of freedom and focuses on quantities that characterize glasses.

First we have a brief review of the Mori-Zwanzig formalism. It says that any time-dependent quantity A obeying the (generalized) Heisenberg equation

$$dA/dt = i\mathcal{L}A \quad (1)$$

also obeys the closed-form equation

$$\dot{A}(t) = i\Omega A(t) - \int_0^t ds K(s)A(t-s) + F(t). \quad (2)$$

The three terms on the RHS are named as the **frequency matrix**, the **memory function**, and the **fluctuating force**, respectively. The fluctuating force collects all “fast” variables that are orthogonal to A , and the memory function is the time autocorrelation function of the fluctuating force. These two terms represent how A gets connected to (in the case in a quantum theory, entangled with) the degrees of freedom that are ignored. Assuming we already have an inner product defined on physical quantities, we have

$$i\Omega = (A, i\mathcal{L}A)(A, A)^{-1}, \quad (3)$$

$$F(t) = e^{it(1-\mathcal{P})\mathcal{L}}i(1-\mathcal{P})\mathcal{L}A, \quad (F(t), A(t)) = 0, \quad (4)$$

and

$$K(t) = -(i\mathcal{L}F(t), A)(A, A)^{-1} = (F(0), F(t))(A, A)^{-1}, \quad (5)$$

where

$$\mathcal{P}X = (A, A)^{-1}(X, A)A. \quad (6)$$

Now we go back to derive a theory about glass transition. The derivation shown below is mainly based on [2].

Viscosity may be viewed as

References

- [1] Liesbeth M. C. Janssen. Mode-coupling theory of the glass transition: A primer. *Frontiers in Physics*, 6, Oct 2018.
- [2] David R Reichman and Patrick Charbonneau. Mode-coupling theory. *Journal of Statistical Mechanics: Theory and Experiment*, 2005(05):P05013, May 2005.
- [3] Wikipedia. Mori-zwanzig formalism. https://en.wikipedia.org/wiki/Mori-Zwanzig_formalism. Accessed: 2021-11-18 09:30:13.