Abstract for the ICTS workshop on Entropic effects in self, driven and directed assembly

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The study of the dynamics of supercooled liquids and glass transition is one of the most active field in modern condensed matter physics. There are many aspects which are studied and one of the interesting areas of investigation is to find the relation between dynamics and structure of glass-forming liquids. In a recent work [1] from our group, it was shown that the structure has the information of the dynamical transition temperature. The dynamics of the system at the pair level was described by independent particles in an external field. The field had the information of the interaction between the particles. It was shown that only structure at pair level is required to describe the field. Using mean first passage time formalism it was shown that for multiple systems the dynamics predicts the dynamical transition temperature. Thus, the formulated theory was successful in differentiating the dynamics of two systems having very similar structure (one where the particles interact via Lennard Jones potential and the other where they interact via the WCA potential) . Although in a similar theory [2, 3] developed by K.Schweizer and later applied [4] by Bertheir and Tarjus it was found that the two systems appear quite similar.

In this work we will analyze why two theories which appear quite similar provide different results. The present work does not attempt to develop a better theoretical framework to study the full dynamics of a supercooled liquid. We employ both the theories to generate their respective results and will compare them in an equitable way.

The basic differences between the two models are in our model we started with a Fokker Planck equation of a binary system and obtained the mean first passage time dynamics on the potential energy landscape. In Scheweizers model they started with the Langevin equation on the Free energy surface of a monatomic system and obtained the dynamics given by Kramers theory. Note that, we can recast any Langevin equation onto a Fokker Planck equation and vice versa. We can also go from mean first passage time (MFPT) dynamics to Kramers dynamics. Thus, the main difference between the two models are ours is the dynamics in the potential energy surface of a binary system and Schweizers is that on the free energy surface of a monatomic system.

TABLE: Results of Systems in Both Method.

System	$T_{\textbf{Nandi } et \textbf{ al.}}$	$\gamma_{\textbf{Nandi } et \textbf{ al.}}$	$T_{\textbf{Schweizer}}$	$\gamma_{\textbf{Schweizer}}$
KALJ	0.4027	40.6093	0.4392	1.4084
KAWCA	0.2820	60.8312	0.2889	3.3981

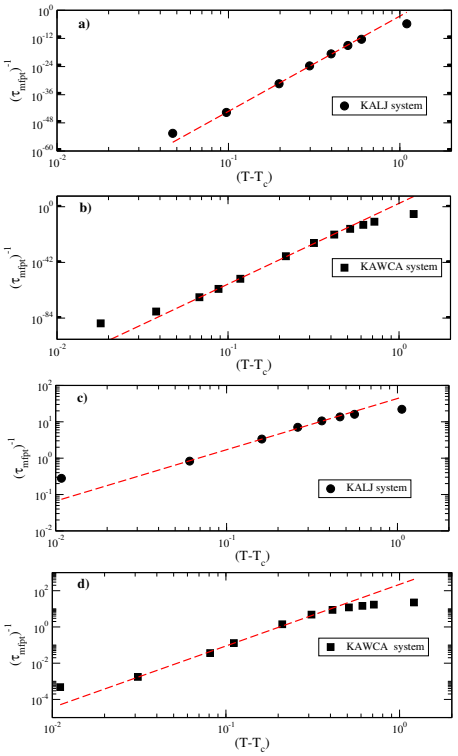

FIG. 1. To show that the present analysis is sensitive to small changes in structure, we compare the results for the Kob-Andersen Lennard-Jones (KALJ) system and its repulsive counterpart the Weeks-Chandler-Andersen (KAWCA) system at $\rho = 1.2$. The power law dependence of $1/\tau_{mfpt}$ predicts a transition temperature T_{mfpt}. Data obtained is given in Table. The dashed lines are the power-law fits. **(a,b)** Analysis of Binary Systems using the methodology developed in Ref [1] (in table as **Nandi *et* al.**), **(c,d)** Analysis of monatomic model systems using Schweizers theory (in Table as **Schweizer**).

It is an ongoing work. However, our preliminary studies indicate that although Schweizer's theory predicts that the dynamics of two systems are not profoundly different; but when analyzed properly we find the dynamical transition temperatures of the two systems are different.

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