

Mermin-Wagner fluctuations in 2D amorphous solids

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While melting in two and three dimension is substantial different, the glass transition in two and three dimensions is usually described with similar methods. Computer simulations recently observed fundamental differences in glassy dynamics, depending on dimensionality. Mermin-Wagner fluctuations can explain such differences without changing the microscopic pictures in 2D and 3D glass.

For structural phase transitions it is well known that the microscopic mechanisms driving the structural changes in two and in three dimensions are not the same. While 3D systems typically show first order transitions with phase equilibrium and latent heat, 2D systems melt via two steps with an intermediate hexatic phase. Unlike in 3D, translational and orientational symmetry are not broken at the same temperature. The scenario is described within the so called KTHNY-theory [1-4] and confirmed e.g. in colloidal monolayers [5]. However, for the glass transition it is usually assumed that dimensionality does not play a role for the characteristics of the transition and 2D and 3D systems are used synonymously. In a recent manuscript, E. Flenner and G. Szamel report fundamental differences of glassy dynamics in two and in three dimensions by large scale computer simulations [6]. They report transient localization to be absent in 2D and translational and orientational correlations times to decouple in 2D but not in 3D.

I propose Mermin-Wagner fluctuations [7,8] (sometimes called Peierls instabilities) to explain the phenomena observed by E. Flenner and G. Szamel. While Mermin-Wagner fluctuations are usually discussed for structural properties they have also impact on dynamical quantities. What are Mermin-Wagner fluctuations? Long before 2D melting scenarios were discussed, there was an intense debate whether crystals and perfect long range order can exist in 1D or 2D at all [9]. A beautiful argument was given by Peierls [9]. Consider a 1D chain of particles with nearest neighbor interaction. The relative distance fluctuation between particle n and particle $n+1$ at finite temperature may be ξ . Similar is the fluctuation between particle $n+1$ and $n+2$. Thus the relative fluctuation between particle n and $n+2$ is $\sqrt{2} \times \xi$ since the relative fluctuations add up *statistically independently* if second nearest neighbor interaction can be ignored. Thus the amplitude of the fluctuations grows with is $\sqrt{N} \times \xi$, if N gives the numbers of particles in the chain. Therefore periodicity cannot exist at large scales in 1D crystals.

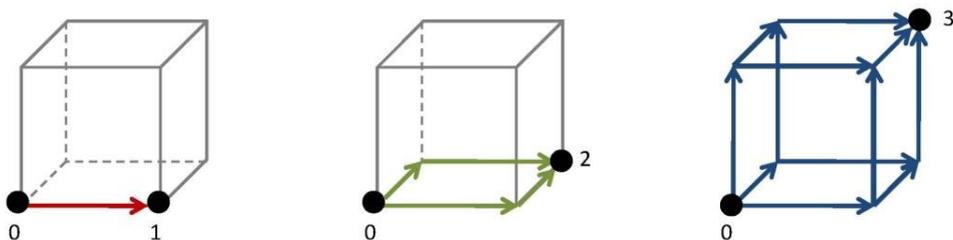


Fig 1: Numbers of ways to cover space in various dimensions. In 1D fluctuations can add up independently while in 3D they have to be correlated along the six different path from 0 to 3.

To cover 3D space one has to investigate three linear independent directions, e.g. within a cube there are six ways to get along the space diagonal say, from the lowest, left, front corner to the upper, right, back corner (see Fig. 1). It follows that in 3D the fluctuations cannot add up independently and the amplitude of the fluctuations stays finite being of the order of ξ . In 2D one can show that fluctuations add up logarithmically at finite temperatures, translational correlation functions decay algebraically while, and this is important to note, orientational order is not affected [7-10].

Mermin-Wagner fluctuations are long(est) wavelength density fluctuations and having a closer look at the arguments [7-10] one finds that periodicity is not a requirement for those fluctuations. They will also be present in an amorphous low dimensional system, provided the fact that a typical particle distance exists (unlike e.g. in a gas). With respect to dynamic measures, Mermin-Wagner fluctuations cause the mean square displacement to diverge in a defect free 2D solid and the standard Lindemann parameter to fail [10,11]. Fig. 2 shows the mean square displacement (MSD) of a hexagonal 2D crystal consisting of ~ 2.000 colloidal particles confined at an interface. The field of view is $620 \times 830 \mu\text{m}^2$ while the whole system is much larger consisting of 300.000 particles. Using local coordinates as introduced by Bedanov, Gadiyak, and Lozovik [12], namely subtracting the trajectories of the nearest neighbors, the so called reduced or local MSD stays finite in a 2D crystal but still diverges in the fluid. This defines a dynamic Lindemann criterion in 2D [12-14]. In the language of glass theory, the nearest neighbors are given by the cage and the ‘cage-relative mean square displacement’ was shown to have much more contrast e.g. for dynamical heterogeneities in a 2D glass former compared to standard displacements [15,16]. It is extreme sensitive to a cage escape process and can measure structural rearrangements but ignores long wavelength fluctuations.

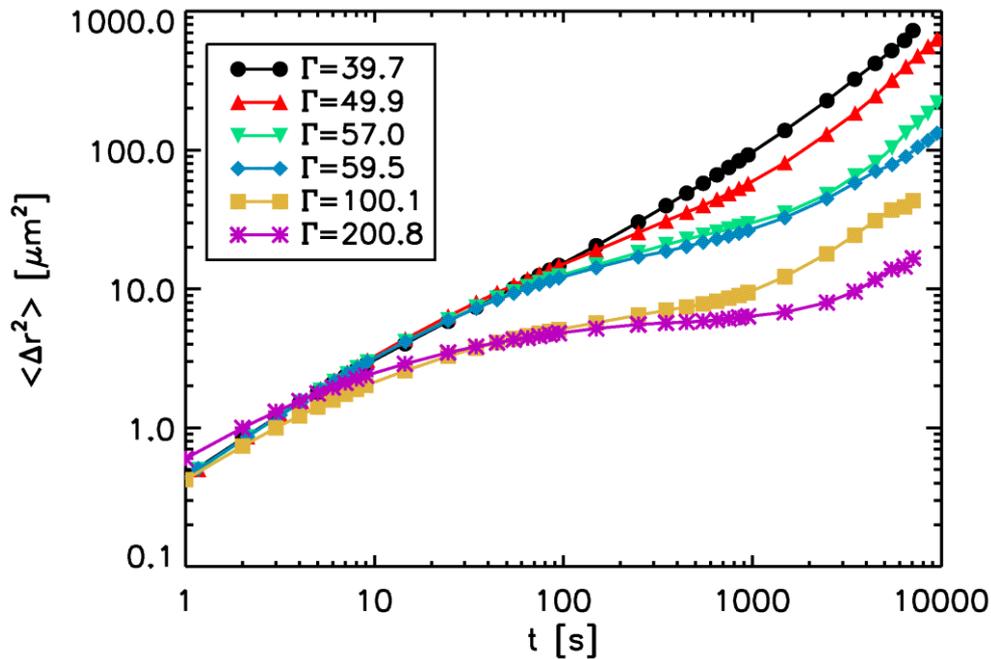


Fig 2: Mean square displacement of a defect free *crystal* (Melting is at $\Gamma = 60$ and the average interparticle distance is about $15 \mu\text{m}$). On large scales and infinite times, even a 2D *crystal* has fluid-like character while using cage-relative coordinates the so called ‘dynamic Lindemann-parameter’ stays finite [11].

Comparing standard MSD and cage relative MSD we observe that Mermin-Wagner fluctuations contribute as an additional diffusive mechanism to the MSD within the α -relaxation. Their existence is not limited to low dimensional *crystals* but will also appear in *amorphous solids* at finite temperatures.

Mermin-Wagner fluctuations can explain the differences in orientational relaxation times (not affected by those fluctuations) and translational relaxations times (affected by those fluctuations) observed by E. Flenner and G. Szamel [6]. Furthermore, Mermin-Wagner fluctuations exist on large scales and the local effect (within the size of the 'cage') is only an affine translation. Thus cage-escape mechanisms and the disappearance of the cage within the fluid are not influenced by Mermin-Wagner fluctuations. Therefore we can conclude that the microscopic mechanism of 2D and 3D glass transition is not necessarily different while the transient localization measured by global variables is less pronounced in 2D compared to 3D.

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