Finite size scaling analysis of the glass transition

Ludovic Berthier

Theoretical Physics, 1 Keble Road, Oxford, OX1 3NP, UK

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We show that finite size scaling techniques can be employed to study the glass transition. Our results follow from the postulate of a diverging correlation length at the glass transition whose physical manifestation is the presence of dynamical heterogeneities. We introduce a parameter $B(T, L)$ whose temperature, $T$, and system size, $L$, dependences permit a precise location of the glass transition. We discuss the finite size scaling behaviour of a diverging susceptibility $\chi(L, T)$. These new techniques are successfully used to study two lattice models. The analysis straightforwardly applies to any glass-forming system.

Progress in the study of the ‘glass transition’ has been slow for two main reasons. First, almost by definition, the dynamics of a liquid supercooled through its melting transition towards its glass phase becomes so slow that it is impossible to actually cross a possible phase transition while staying at equilibrium. One relies therefore on thermodynamic or kinetic extrapolations which stop at the glass temperature $T_g$ where the system no longer equilibrates. As a consequence, the mere existence of a genuine transition is still questioned, even though experiments now probe more than a decade of decades of relaxation times.

Secondly, the nature of the putative transition remains largely unknown as compared to more standard phase transitions. Basically, the situation is such that the formulation of a Ginzburg-Landau type of model is still impossible, because one does not know what would be the correct order parameter, its symmetries, dynamics, correlations, etc. Similarly, at the beginning of the 90’s, two papers apparently settled the related question of the possible existence of a diverging correlation length at the glass transition, reporting the absence of such a length scale. As a regrettable corollary, modern developments of statistical mechanics such as renormalization group, finite size scaling, or universality classes became apparently useless to study the glass transition.

In this paper, we show that finite size scaling techniques first derived from renormalization group concepts in the context of continuous phase transitions are useful to study the glass transition, at variance with the common belief. This should allow much more powerful extrapolations to locate a possible transition and a better characterization of its nature, thus making progress on the two important points mentioned above.

The paper is organized as follows. We first describe the observations underlying our work, before describing the principles of the analysis. As a first application of the method, we then consider two well-known models proposed in the context of the glass transition, namely the one-dimensional Fredrickson-Andersen model and the three-dimensional Kob-Andersen model.

Our work is based upon the recent burst of activity related to the definition, observation and characterization of dynamical heterogeneities in the dynamics of supercooled liquids. The underlying physics is that particles move in a cooperative manner, the more so the nearer the glass transition. This picture immediately suggests the existence of a correlation length $\xi(T, t)$ associated to these dynamical domains, reflecting the length scale on which the particles dynamics have been correlated in a time interval $t$ at temperature $T$. We define a ‘coherence length’ $\ell(T) \equiv \xi(T, t_{rel})$, where $t_{rel} = t_{rel}(T)$ is the mean relaxation time of the liquid. Whether or not $\ell(T)$ is connected to some yet undiscovered structural length scale is an important open problem. Crucially, however, progress can be made if one postulates that $\ell(T)$ actually diverges at some—possibly zero—temperature $T_c$ which will thus non-ambiguously define the glass transition temperature one seeks to determine. It should coincide with the temperature at which $t_{rel}(T)$ also diverges.

A measure of $\xi(T, t)$ in a liquid can be obtained via the spatial decay of the following correlation function:

$$C(r, t) = \langle F(r + r_0, t)F(r_0, t) \rangle - \langle F(r + r_0, t) \rangle \langle F(r_0, t) \rangle,$$

where $F(r, t) = \rho(r, t + t_0)\rho(r, t_0)$; $\rho(r, t)$ is the density at time $t$ and position $r$, $r_0$ and $t_0$ are arbitrary position and time, respectively. Alternatively, $F(r, t)$ can be replaced by any two-time function, $F(r, t) = A(r, t + t_0)B(r, t_0)$, where $A$ and $B$ are physical observables. In essence, Eq. 1 is a two-time, two-point correlation function which measures correlations in trajectory space. Note that the commonly discussed ‘non-Gaussian parameter’ is related to Eq. 1 when $A$ and $B$ refer to the particle positions, but for $r = 0$. As such, it contains no information about $\ell(T)$. In fact, Eq. 1 captures most of the measurements of dynamical heterogeneities which amounts to first distinguish between ‘fast’ and ‘slow’ particles and then to check how these are spatially correlated. The correlators $F(r, t)$ precisely tell us how fast a particle is, while Eq. 1 measure the corresponding spatial correlations. The use of the dynamic function $F(r, t)$ makes an arbitrary criterion to distinguish...
between particles unnecessary. Variations of the correlator have been studied. In Refs. [8, 11], the density fluctuations were replaced by an arbitrarily defined overlap between configurations, and by particle displacements in Refs. [3, 14, 11]. These works show that \( \xi(T, t) \) is indeed maximum for \( t \approx t_{\text{rel}}(T) \), which justifies our definition of \( \ell(T) \). Also, \( \ell(T) \) decreases with \( T \), although simulations are yet too limited to confirm a possible divergence at low temperature.

The observation of a growing coherence length scale has deep consequences which we start to explore in this paper. This indeed suggests that local dynamical functions \( F(r, t) \) become long-range correlated when the glass phase is approached. As such they play a role similar to that of the order parameter in a standard continuous phase transition. This simple remark is central in our approach. Having identified a quantity analogous to an order parameter, it becomes a simple task to extend the tools developed for conventional transitions to study the problem of the glass transition, starting here with finite size scaling techniques.

Define first the parameter \( B(T, L) \) as

\[
B(T, L) = 1 - \frac{\langle \varphi^4 \rangle_L - 4\langle \varphi^3 \rangle_L \langle \varphi \rangle_L + 6\langle \varphi^2 \rangle^2_L - 3\langle \varphi \rangle^3_L}{3\langle \varphi^2 \rangle^2_L - 2\langle \varphi^2 \rangle L \langle \varphi \rangle^2 + \langle \varphi \rangle^4_L} \tag{2}
\]

with \( \varphi = \varphi(t_{\text{rel}}(T)) \equiv L^{-d} \int d^d F(r, t_{\text{rel}}(T)) \), where \( d \) is the space dimensionality. The crucial information is that the average \( \langle \cdots \rangle_L \) is performed in a system of finite linear size \( L \). By construction, \( B(T, L) = 0 \) when the fluctuations of \( \varphi \) are Gaussian, since it is built from the fourth cumulant of the probability distribution function of \( \varphi \), \( P_L(\varphi) \). This distribution is Gaussian when \( L \gg \ell(T) \) as a consequence of the central limit theorem. However, \( P_L(\varphi) \) becomes non-Gaussian when \( L < \ell(T) \), and \( B(T, L) \) is therefore non-zero in that case. Moreover, it is natural to expect that \( B(T, L) \) becomes a scaling function of the variable \( \ell(T)/L \) in the regime \( \ell(T), L \gg a \), where \( a \) is the microscopic length scale of the problem, e.g. the particle size in a simple liquid. Also, \( P_L(\varphi) \) should be independent of \( L \) and \( \ell(T) \) in the regime \( a \ll L \ll \ell(T) \).

The latter assumption implies in particular that \( B(T_c, L) \) is a constant ‘universal’ number since \( L \ll \ell(T_c) = \infty \) is automatically satisfied at the transition. Therefore, the curves \( B(T, L) \) versus \( T \) for various \( L \) cross at \( T_c \). The definition (2) is naturally inspired by the classical paper [12], where a numerical finite size scaling analysis of the Ising model was performed. In that case, \( \varphi \) was the order parameter of the paramagnetic-ferromagnetic transition, i.e. the magnetization density.

We also define the susceptibility

\[
\chi(T, L) = \frac{L^d}{T} \left[ \langle \varphi^2 \rangle_L - \langle \varphi \rangle^2_L \right], \tag{3}
\]

again explicitly retaining its \( L \) dependence. Similarly, one expects this function to exhibit a scaling behaviour for large \( L \) and \( \ell(T) \). When the correlator \( C(r, t) \) is itself a simple function of the ratio \( r/\ell(T) \), one gets

\[
\chi(L, T) \approx L^d \tilde{\chi} \left( \frac{\ell(T)}{L} \right), \tag{4}
\]

where the scaling function \( \tilde{\chi}(x) \) behaves as \( \tilde{\chi}(x \ll 1) \approx x^\gamma \) and \( \tilde{\chi}(x \gg 1) \approx \text{const} \). The assumption made on the correlator is supported by all known simulation results so far [8, 14, 11]. It is satisfied also in the two models studied below. Using with caution the language of critical phenomena, this would mean that the anomalous exponent \( \eta \) is \( \eta = 2 - d \), implying a simple Fisher’s law \( \gamma = \nu d \) between the exponents of the susceptibility and the correlation length. This point certainly needs further investigation in realistic supercooled liquids.

The suggested analysis requires extrapolations towards the glass phase, as all equilibrium measurements in supercooled liquids do. However, the new quantities \( B(T, L) \) and \( \chi(T, L) \) defined above are much richer quantities than, say, an average relaxation time since they contain information on the full distribution \( P_L(\varphi) \). This will be clearly demonstrated in the rest of the paper.

We now use the analysis suggested above to study two lattice models. We start with the one-dimensional version of the spin facilitated Ising model introduced in Ref. [3]. Spin facilitated models have been introduced as caricatures of real supercooled liquids, in the sense that they are non-disordered spin models displaying glassy dynamics with only very simple static correlations. We have chosen this version of the model since it is reasonably well characterized [3, 14, 15]. Moreover, as a one-dimensional lattice model, it is relatively easy to simulate on very large time and length scales, nicely confirming the expected scaling behaviour. These results thus constitutes a very interesting first application of the methods de-
whose value is 1. This kinetic constraint implies glassi-
spin can flip only if it has at least one nearest neighbor
the density of spin 1 becomes small at low
allowing less and less transitions. This leads to an Arrhe-
ent configurations ranging from 200 to 20000. Fortu-
the inverse temperature $1/T$ for the same sizes as Fig. 1
increasing from bottom to top. Main: The rescaled sus-
ceptibility $\chi(T, L)L^{-1}$ as a function of the scaling variable
log$(\ell(T)/L)$ with $\ell(T) = \exp(1/T)$. Both figures are for the
one-dimensional spin facilitated Ising model.

described above. The model is defined by the Hamiltonian

$$H = \sum_{i=1}^{N} s_i,$$

where $s_i = 0, 1$ are two-state observables located at the
sites of a chain of size $N$ with periodic boundary condi-
tions. Glassiness originates from the chosen dynamics,
since the static properties of the non-interacting Hamil-
tonian 5 are completely trivial. In a standard Metropo-
olis algorithm, the transition rates are $w(s_i \to 1 - s_i) = \min(1, e^{-\beta \Delta E})$, where $\Delta E$ is the energy change in
the transition $s_i \to 1 - s_i$. Here, the rates are given in-
stead by $w'(\Delta E) = (s_{i-1} + s_{i+1})w(\Delta E)$ meaning that a
spin can flip only if it has at least one nearest neighbor whose value is 1. This kinetic constraint implies glassi-
ness. From 5, one has $\langle s_i \rangle = \left(1 + e^{1/T}\right)^{-1}$, so that the
density of spin 1 becomes small at low $T$ therefore allowing less and less transitions. This leads to an Arrhe-
nius relaxation time, $t_{rel} = \exp(3/T)$, which makes the model ‘strong’ according to the classification commonly
used in the glass literature. Also, the dynamics becomes more and more cooperative when approaching the glass transition at $T_c = 0$, with a diverging coherence length
$\ell(T) = \exp(1/T)$.

We simulate this model using a continuous time algo-
rithm in the temperature interval $T \in [0.125, 1.0]$, ap-
proximately corresponding to 13 decades in relaxation
times. For each temperature, a large system of $N = 2 \cdot 10^4$
spins is studied, and averages are performed in subsys-
tems of finite size $L \in [2, 1024]$ for a number of independent
configurations ranging from 200 to 20000. Fortu-
nately, more statistics is required at higher temperatures
where deviations from Gaussian behaviour are smaller. A natural choice for the dynamic function $F(i, t)$ in the
definition 2 is the persistence of the spin $s_i$ at site
$i$. The mean persistence is given by $(F(i, t))_{t=\infty} = \exp\left(-\sqrt{t/t_{rel}(T)}\right)$, which defines the relaxation time.

Our results for this model are presented in Figs. 1 and
2. The inset of Fig. 1 shows the variation of $B(T, L)$
as a function of $1/T$ for various sizes $L$. As expected,
$B(T, L)$ crosses over from $B(T, L) = 0$ at high $T$ to a
non-zero value at low $T$, the locus of the crossover being
$L$-dependent. The various curves clearly cross at $T_c = 0$
only. One observes in the main figure an excellent col-
lapse of the data, showing that $B(T, L)$ satisfies the ex-
pected scaling form $B(T, L) \approx B(\ell(T)/L)$. Since $P_L(\phi)$
is bimodal when $L \ll \ell(T)$, it is a simple task to com-
pute $B(T_c = 0, L) = B(x \to \infty) = 0.566...$. The inset of Fig. 2 presents the susceptibility $\chi(T, L)$ as a function of
$1/T$ for various sizes $L$. Again, one clearly sees the ex-
pected behaviours: $\chi(T, \infty)$ diverges when $T \to 0$ as
$e^{1/\ell(T)} = \ell(T)$, while for finite $L$ the divergence is smeared
when $\ell(T) > L$. The main figure shows the perfect col-
lapse of the data suggested by Eq. 3 when $\chi(L, T) L^{-1}$
is plotted as a function of $\ell(T)/L$ (remember that $d = 1$).

As a second application of the techniques described
above, we study the kinetically constrained lattice gas
introduced in Ref. 8. The model consists of hard spheres
on a cubic lattice of linear size $N$. In this case, tem-
perature plays no role, and the relevant control param-
eter is the density of particles, $\rho$. This lattice gas is
also complemented by kinetic rules which make the dy-
namics glassy. In a non-constrained lattice gas, particles
move to an empty nearest neighbour site with unit rate.
In the present model, particles can move to an empty
nearest neighbour, provided the particle has fewer than 4
neighbours before and after the move. This kinetic
rule aims at reproducing dynamics of a supercooled liq-
uid, where particles can hardly escape the cage formed
by their neighbours. As a simple lattice model for the
glass transition, it has been much studied since its intro-
duction. Simulations have reported a dynamical arrest
at a density $\rho_c \approx 0.881$ where the relaxation time appar-
ently diverges as a power law 8. Very recently, however, a
lower bound for the diffusion constant was analytically
derived for this model, showing that the divergence of the
relaxation time at a finite density found in simulations is
only apparent 14. The growth of $t_{rel}(\rho)$ with $\rho$ is in fact
extremely abrupt, $\log \log t_{rel}(\rho) \propto (1 - \rho)^{-1}$, with an
associated coherence length $\log \log \ell(\rho) = c/(1 - \rho)$, where $c$
is a numerical constant. The extremely fast increase of $t_{rel}$ can easily be numerically confused with a true
divergence at a finite density. This more difficult problem
represents thus a highly selective test for the methods
described in this paper. We now show that finite size
scaling allows one to distinguish between a true and an
apparent divergence of the relaxation time in this model.

We use again a continuous time Monte Carlo algorithm
to study a model of linear size $N = 24$ for densities
The parameter $B(T, L)$ as a function of the reduced variable $\log(\ell(\rho)/L)$ with $\ell = (\rho_c - \rho)^{-\alpha}$ (top) or $\ell = \exp\exp(c/(1 - \rho))$ (bottom). A much better collapse is obtained in the bottom part, with only one free parameter. Systematic deviations are visible in the top part. Both are for the kinetically constraint lattice glass of Ref. [4].

To summarize, we have shown that finite size scaling techniques can be used to study the glass transition. This follows from the identification of local two-time observables $F(r, t)$ as relevant 'order parameters' with interesting fluctuations and correlations. We have defined two quantities, $B(T, L)$ and $\chi(T, L)$, whose scaling behaviour allows one to locate the glass transition in a much more accurate manner than an extrapolation of simpler quantities such as the relaxation time. The method proposed here straightforwardly applies to any glass-forming systems, including off-lattice models. More generally, our results show that the glass transition has more in common with continuous phase transitions than usually believed and raise the hope that more concepts and methods borrowed from continuous phase transitions studies can also be used.

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