Ideal glass transitions for hard ellipsoids.

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For hard ellipsoids of revolution we calculate the phase diagram for the idealized glass transition. Our equations cover the glass physics in the full phase space, for all packing fractions and all aspect ratios $X_0$. With increasing aspect ratio we find the idealized glass transition to become primarily be driven by orientational degrees of freedom. For needle or plate like systems the transition is strongly influenced by a precursor of a nematic instability. We obtain three types of glass transition lines. The first one ($\phi_c^{(B)}$) corresponds to the conventional glass transition for spherical particles which is driven by the cage effect. At the second one ($\phi_c^{(B')}$) which occurs for rather non-spherical particles a glass phase is formed which consists of domains. Within each domain there is a nematic order where the center of mass motion is quasi-ergodic, whereas the inter–domain orientations build an orientational glass. The third glass transition line ($\phi_c^{(A)}$) occurs for nearly spherical ellipsoids where the orientational degrees of freedom with odd parity, e.g. $180^\circ$ flips, freeze independently from the positions.

I. INTRODUCTION

The dynamics of a molecular system which is supercooled towards the glass transition shows a variety of phenomena related to the nontrivial interplay between orientational and translational degrees of freedom caused, e.g. by steric hindrance. Already in thermodynamic equilibrium molecular systems show, compared to simple liquids, a variety of different physical behavior. At low enough densities (or high enough temperatures) they form an isotropic liquid. On increasing the density they can undergo a transition into a crystal or several different liquid crystalline phases (like a nematic phase). A crucial part of the interaction which causes these phenomena is given by the shape of the molecules. Therefore one may also expect new characteristic features for the glass transition in such systems. A model system which allows to study the translation–orientation interplay is a system of $N$ hard ellipsoids of revolution in a box of volume $V$. The fluid of ellipsoids is characterized by two parameters: The aspect ratio $X_0 = \frac{b}{a}$ relating $b$ and $a$, the major and minor axis of the ellipsoids, and the packing fraction $\phi$ which is related to the number density $\rho = \frac{\phi}{V}$ by $\phi = \frac{4}{3} \pi X_0 \rho$.

In this work we start from a theory of liquids. We demonstrate that a single set of equations allows to describe the glassy behavior for almost spherical particle up to large aspect ratios where pre-nematic order becomes crucial.

The choice of the model system has also been motivated by the successful application of the ideal mode coupling theory (MCT) for simple liquids [9], particularly to neutral colloidal suspensions. MCT gives a closed set of equations for the intermediate scattering function $S(q, t)$. Comparison between experimental [2] and MCT–results [10] have shown good agreement for the colloidal systems which usually are modeled by hard spheres. Further tests of the MCT for other systems can be found in e.g. refs. [2–8]. MCT in its original form describes an idealized glass transition which is indicated by breaking of ergodicity, at a critical density $\rho_c$ (or critical temperature $T_c$). The corresponding non-ergodicity parameter $f(q) = \lim_{t \to \infty} S(q, t)/S(q, 0)$ becomes nonzero at $\rho_c$ (or $T_c$). Recently the mode coupling equations have been extended to molecular systems. The dynamics of liquids of rigid molecules composed of $M$ atoms can either be described by site–site correlators $S_{\alpha,\beta;\alpha,\beta} = 1, 2, ..., M$ or molecular correlation functions $S_{lmn,l'm'n'}(q, t)$ where for the latter one decomposes the degrees of freedom into the center of mass and orientational components (see e.g. [2,8]). The density $\rho(x, \Omega, t)$ is a function of the center of mass coordinate $x$ and the orientation $\Omega = (\Phi, \theta, \chi)$ which is specified by the three Euler angles. Expanding $\rho(x, \Omega, t)$ with respect to a product basis of plane waves, $e^{i\mathbf{x} \cdot \mathbf{r}}$ and generalized spherical harmonics $D_{lmn}(\Omega)$ one arrives at the tensorial density $\rho_{lmn}(q, t)$. $l$ runs over all positive integers including zero and $m$ and $n$ takes integer values between $-l$ and $l$. Then the molecular correlators are defined as follows:

$$S_{lmn,l'm'n'}(q, t) = \frac{1}{N} \langle \rho_{lmn}^*(q, t) \rho_{l'm'n'}(q, 0) \rangle$$

The extension of MCT to molecular systems has been done for the molecular representation for a single dumbbell in a simple, isotropic liquid [9], for molecular liquids of linear molecules [11] and for arbitrarily shaped molecules by use of nonlinear fluctuating hydrodynamics [12] and by Mori–Zwanzig projection formalism [13]. An MCT–approach using a site–site description has recently been worked out [14]. Because a hard ellipsoid corresponds to a rigid body with infinitely many constituents it is the molecular representation which is the only appropriate one. Since we consider ellipsoids of revolution the third Euler angle $\chi$ becomes redundant. This means that we have to consider $S_{l00,l'm'0}(q, t)$, only. Using the $q$-frame [9], i.e. one chooses $q = (0, 0, q) \equiv q_0$ where
\[ q = |q| \text{, these correlators become real and diagonal in } m \text{ and } m' \text{[10]}:\]

\[ S_{l,m_0,t',m_0}(q, t) = \delta_{m,m'} S_{l}(q, m, t) \quad . \tag{2} \]

The head–tail symmetry of the ellipsoids implies that these correlators vanish for \( l + l' \) odd. For given \( X_0 \) the critical packing fraction \( \phi_c(X_0) \) can be determined by calculating the (unnormalized) non-ergodicity parameters \( F_{l'}(q, m) = \lim_{t \to \infty} S_{l}(q, m; t) \).

\section*{II. MOLECULAR MODE-COUPLING EQUATIONS}

Using the densities \( \rho_{lm}(q, t) \) and longitudinal translational currents \( j^{l}_{lm}(q, t) \) and rotational currents \( j^{l'}_{lm}(q, t) \) as slow variables set for the Mori-Zwanzig projection operator technique the molecular MCT–equations have been derived and can be found in refs. [10] and [12].

The time dependent molecular MCT–equations can be represented as follows:

\[
\frac{\partial}{\partial t} S(q, m, t) = N^{R}(q, m, t) + N^{T}(q, m, t) \\
\frac{\partial}{\partial t} N^{\alpha}(q, m, t) = -\Omega_{\alpha}^{2}(q, m) S(q, m, t) \\
\quad - \sum_{\alpha'} \nu_{\alpha\alpha'}(q, m) N^{\alpha'}(q, m, t) \\
- \Omega_{\alpha}^{2}(q, m) \sum_{\alpha'} \int_{0}^{t} m^{\alpha,\alpha'}(q, m, t - t') N^{\alpha'}(q, m, t) d' \quad (3)
\]

and:

\[
m^{\alpha,\alpha'}_{l,l'}(q, m, t) = \sum_{\alpha = \{T, R\}} \sum_{m_1} \sum_{m_2} V^{m_1,m_2,\alpha,\alpha'}_{l,l',l_2,l_2'}(q, q_1, q_2) \\
S_{l_1,l_2'}(q_1, m_1, t) S_{l_2,l'_2}(q_2, m_2, t) \quad (4)
\]

The indices \( \alpha, \alpha' \in \{T, R\} \) refer to either translational or rotational currents while \( \Theta_T \text{ and } \Theta_R \text{ are the mass and moment of inertia, respectively. } N^{\alpha}(q, m, t) \) are the current–density correlation functions for translational \( (\alpha = T) \) and rotational \( (\alpha = R) \) currents multiplied with \( q \text{ and } \sqrt{l(l+1)} \), respectively. The microscopic frequency matrix is denoted by \( \Omega_{\alpha}(q, m) \) and is determined by the static molecular correlators. In the absence of memory effects \( (m^{\alpha,\alpha'} = 0) \) the equations are just a set of coupled harmonic oscillators with friction \( \nu_{\alpha\alpha'} \) for vibrational \( (\alpha = T) \) and rotational \( (\alpha = R) \) oscillations.

E.g. the translational mode with \( l = l' = 0 \) is the propagating phonon mode and the modes with \( l = l' > 0 \) which exhibit a frequency gap at \( q = 0 \) are localized oscillators.

For \( m^{\alpha,\alpha'} \neq 0 \) nonlinearities occur. Their physical origin are memory effects. The corresponding memory kernel is a correlation function of fluctuating forces. Since fluctuating forces can decay into a pair of density excitations this kernel is approximated as a sum of all possible \textit{bilinear} products of density correlation functions. Such a non–linear feed back mechanism can cause an ideal glass transition with non–trivial dynamics. The glass transition for eqs. (3) and (4) is investigated in the following part of the paper. The explicit expressions for the vertices \( V^{\alpha\alpha'} \) for arbitrary \( q \) can be found in ref. [10] and for the q-frame in ref. [12]. The vertices \( V^{\alpha\alpha'} \) only depend on the static correlators \( S_{l}(q, m) \) and the direct correlation function \( c_{l'}(q, m) \) which are related to each other by the Ornstein–Zernike equation. We have determined \( c_{l'}(q, m) \) within Percus–Yevick approximation.

It has been shown that the liquid phase of hard ellipsoids is well described by these approximations [14]. Although Percus–Yevick theory fails to describe crystallization it yields a nematic instability [3] which is in reasonable agreement with Monte–Carlo simulations [3] even if Percus–Yevick theory still underestimates the tendency towards orientational order. This nematic instability will play an important role in the following. For the solution of the Percus–Yevick equations we have chosen a cut–off \( l_{co} = 4 \) for \( l \text{ and } l' \), whereas the MCT equations were truncated at \( l_{co} = 2 \). We are confident that even such a small number of molecular correlators enables us to capture the correct physics of the transition.

\section*{III. SOLUTION OF THE MMCT FOR HARD ELLIPSOIDS}

The numerical solution of the eqs. (3)-(4) for \( t \to \infty \) yields the non-ergodicity parameters \( F_{l'}(q, m) = \mathbf{F}(q, m) \). In the limit of \( t \to \infty \) the following set of nonlinear equations for \( \mathbf{F}(q, m) \) has to be solved in an iterative way:

\[
\sum_{\alpha\alpha'} q^{\alpha}_{l}(q)q^{\alpha'}_{l}(q) \left( \mathcal{F}(q, m)^{-1} \right)^{\alpha\alpha'} S^{-1}(q, m) \mathbf{F}(q, m) + \mathbf{F}(q, m) - \mathbf{S}(q, m) = 0 \quad (5)
\]

\[
\mathcal{F}_{l,l'}^{\alpha,\alpha'}(q, m) = \sum_{q_1, q_2} \sum_{m_1} \sum_{m_2} \sum_{i_1, i_2} \sum_{i'_1, i'_2} \nu^{m_1,m_2,\alpha,\alpha'}_{l,l',i_1,i_2,i'_1,i'_2} \mathcal{F}_{l_1,l_2'}(q_1, m_1) \mathcal{F}_{l_2,l'_2}(q_2, m_2) \quad (6)
\]

The indices \( \alpha, \alpha' \in \{T, R\} \) refer to either translational or rotational currents while \( \Theta_T \text{ and } \Theta_R \text{ are the mass and moment of inertia, respectively. } N^{\alpha}(q, m, t) \) are the current–density correlation functions for translational \( (\alpha = T) \) and rotational \( (\alpha = R) \) currents multiplied with \( q \text{ and } \sqrt{l(l+1)} \), respectively. The microscopic frequency matrix is denoted by \( \Omega_{\alpha}(q, m) \) and is determined by the static molecular correlators. In the absence of memory effects \( (m^{\alpha,\alpha'} = 0) \) the equations are just a set of coupled harmonic oscillators with friction \( \nu_{\alpha\alpha'} \) for vibrational \( (\alpha = T) \) and rotational \( (\alpha = R) \) oscillations.

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\[
\mathcal{F}(q, m) = \lim_{z \to 0} -z m^{\alpha,\alpha'}(q, m, z) = \lim_{t \to \infty} m^{\alpha,\alpha'}(q, m, t) \text{ we denote the long time limit of the memory kernel. From a solution of these equations we obtain the phase diagram for ideal glass transitions which is shown in fig. 4. Figure also contains two dashed–dotted lines } \Phi_{sem}(X_0) \text{ indicating the location of the nematic instability as it arises in}
\]
continuous (also called type–A) glass transition occurs at a density (e.g. from Monte–Carlo simulations \[^{15}\]) resulting from a Maxwell construction. The two densities (e.g. from Monte–Carlo simulations \[^{15}\]) are in agreement with density functional theory \[^{14}\]. The existence of \(\phi_c^{(B)}(X_0)\) has been established for 0.35 \(< X_0 < 2.5\). In the region where the \(\phi_c^{(B)}(X_0)\) glass transition occurs the equilibrium system shows crystallization. Being a first order phase transition the onset of crystallization gives two densities (e.g. from Monte–Carlo simulations \[^{15}\]) resulting from a Maxwell construction. The \(\phi_c^{(B)}(X_0)\) glass transition line is well bracketed between these two densities. This indicates that the mode coupling equations describe a glass transition in the meta-stable region of a super-cooled liquid. The physical origin of the glass transition depends strongly on the location on \(\phi_c^{(B)}(X_0)\).

For aspect ratios \(X_0\) close to one the transition is dominated by the center of mass correlator \(S_{00}(q,0)\). To illustrate this point we have plotted in fig. \[^{2}\] the static center of mass correlator and the “quadrupolar” correlator \(S_{22}(q,0)\) and their corresponding non–ergodicity parameters for \(X_0 = 1.3\). This was done directly above the critical packing fraction \(\phi_c = 0.549\). The first peak at \(q_{\text{max}} = q \approx 6.6\) \(a^{-1}\) of \(S_{00}(q,0)\) dominates the transition which is the manifestation of the cage effect. Stronger deviations of the ellipsoids from spherical symmetry, however, alter this behaviour. This is demonstrated in fig. \[^{3}\] where we have plotted the same correlators as in fig. \[^{2}\] but for an aspect ratio of \(X_0 = 2.3\). Now the peak at \(q \approx 0\) of the quadrupolar correlator \(S_{22}(q,0)\) (which is for \(q=0\) the Kerr constant for non polar fluids) dominates the breaking of ergodicity. The half width \(\Delta q\) (at half maximum) of this peak defines a correlation length \(\xi = 2\pi/\Delta q\). In fig. \[^{3}\] we have plotted \(\xi\) at the glass transition line (either \(\phi_c^{(B)}\) or \(\phi_c^{(B')})\) as a function of the aspect ratio \(X_0\) for prolate ellipsoids.

Within the glassy phase, i.e. for \(\phi > \phi_c^{(B)}(X_0)\) a continuous (also called type–A) glass transition occurs at the critical lines \(\phi_c^{(A)}(X_0)\) (thin solid lines) at which the vertex \(V\) is large enough. To this happen the aspect ratio should clearly be different from one. The reader should note that four points (open circles) were determined exactly and the thin solid line is schematic, showing that \(\phi_c^{(A)}(X_0)\) has to increase if \(X_0\) is changed towards one, in order to keep the vertices large enough. The physical interpretation is that at \(\phi_c^{(A)}(X_0)\) the 180°–jumps of the ellipsoids become frozen. This resembles the formation of orientational glasses. One possible candidate for such a transition might be plastic crystals like the carboranes \[^{17}\] although presently only type B transitions are detected.

Probably the most interesting result is the third critical line \(\phi_c^{(B')} (X_0)\) (dashed line) which is shown schematically in fig. \[^{5}\] for \(X_0 > 2.0\) (prolate ellipsoids) and \(X_0 < 0.5\) (oblate ellipsoids). In this region the glass transition lines are close to the nematic instability line. The existence of \(\phi_c^{(B')} (X_0)\) is based on our following observations. Increasing \(\phi\) for \(2.1 < X_0 < 2.5\) we find a glass transition at \(\phi_c^{(B)}(X_0)\) where all \(F_{ll}^{\prime}(q,m)\) become nonzero. Increasing \(\phi\) further we find in addition a second solution \(F_{ll}^{\prime}(q,m)\) for \(\phi \geq \phi_c^{(B)}(X_0)\). This solution has the feature that \(F_{ll}^{\prime}(q,m)\) is practically zero with the exception of a well pronounced peak for \(F_{22}^{\prime}(q,m)\) at \(q = 0\) and with a width of order \(\xi\). We have shown this in fig. \[^{5}\] where we have plotted \(F_{22}^{\prime}(q,0)\) at the \(\phi_c^{(B')}\) transition for \(X_0 = 2.5\). This is plotted together with the static correlator \(S_{22}(q,0)\) and the normalized function \(F_{22}^{\prime}(q,0) = F_{22}^{\prime}(q,0)/S_{22}(q,0)\). In fig. \[^{5}\] we have plotted the same quantities for \(l = l' = 0\), the center of mass correlator, \(F_{00}^{\prime}(q,0)\) does not exceed 0.15 although the orientations are frozen. This means that the system is “quasi–ergodic” in the sense that for length scales \(l \ll \xi\) the ellipsoids show a (nematic) orientational order and the center of mass behaves “quasi–ergodic” decaying to a very small value. Whereas for length scales \(l \gg \xi\) the orientations as well as the positions have non–decaying, long–time correlations and are frozen. The easiest way to think of such a system is due to the formation of liquid crystalline (nematic) domains with a size of the order of \(\xi\). This is visualized in fig. \[^{5}\] in fig. \[^{5}\] shows that the domains can be quite large. For \(X_0 = 2.5\) (the aspect ratio where the type–B’ transition occurs first and where therefore the type–B’ transition with the smallest domain size shows up) we obtain from our calculation a domain size with \(\xi \approx 30\). Within the domains the center of mass is “quasi–ergodic” i.e. liquid like whereas the orientations are frozen with a nematic order. In our idealized MCT an ellipsoid can not move from one domain to the other.

In connection with this it is also interesting to mention that two types of type B transitions were also found for the center of mass correlator of a simple liquid of hard spheres with an attractive interaction given either by the Baxter model \[^{18}\] or a Yukawa potential \[^{19}\]. The existence of these two solutions for \(X_0 > 2.1\) reflects the competition between the frozen positional disorder due to the cage effect and the tendency to form a nematic phase. Since \(F_{ll}^{\prime}(q,m) < F_{ll}(q,m)\) for \(2.1 < X_0 < 2.5\) the second solution is unphysical \[^{17}\]. However, for \(X_0 \geq 2.5\) and \(\phi_c^{(B')} (X_0) \leq \phi \leq \phi_{\text{nem}}(X_0)\) we only find one solution which has all the features of \(F_{ll}^{\prime}(q,m)\) described above. We stress that the existence of the critical line \(\phi_c^{(B')} (X_0)\) trusts on our choice of slow variables which includes the nematic order parameter and therefore accounts for the occurrence of the weakly first order nematic transition. Since \(\phi_c^{(B')} (X_0)\) is rather close to \(\phi_{\text{nem}}(X_0)\)” quasi–critical” fluctuations appear which
also slow down the entropy fluctuations. We do not think that those will qualitatively change the phase diagram. On the other hand the concept of a glass transition induced by the vicinity of a second order phase transition was already introduced by a MCT approach \cite{21} in order to describe the experimentally observed central peak phenomenon close to a ferroelectric instability.

IV. CONCLUSION

In conclusion, we have shown that hard ellipsoids exhibit a rather intriguing phase diagram obtained from the idealized mode coupling theory for molecular systems, where the orientational degrees of freedom and their coupling to translational ones is incorporated. Particularly, we predict a glass transition for \( X_0 > 2 \) which is driven by a precursor of a nematic phase. Ellipsoids show two type-B glass transition lines \((\phi_{c}^{(B)} \) and \( \phi_{c}^{(B')} \)). One, \( \phi_{c}^{(B)} \), is dominated by the cage effect whereas the other one \( \phi_{c}^{(B')} \) is caused by an orientational (nematic) instability. Besides this a type-A glass transition occurs for almost spherical ellipsoids where the orientational degrees of freedom with odd parity, e.g., \( 180^\circ \)-flips freeze independently from the translational ones. It would be very interesting to check these predictions by experiments or simulations.

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[20] It was proven in \cite{4} that the largest solution of the non linear MCT equations is the physical one. It is not clear whether this can be extended to molecular liquids. However we have found that \( F_{11}^{(q,m)}(q,m) < F_{11}(q,m) \) for all \( q,m \) and \( l = l' \leq 2 \), it is tempting to believe that it is still true.
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FIG. 1. Phase diagram for the ideal glass transitions. The horizontal axis shows \( X_0 \) scaled with \( \frac{X_0^2}{X_0^2} \). The type-B glass transition lines \( \phi_{c}^{(B)}(X_0) \) and \( \phi_{c}^{(B')}(X_0) \) (see text) are depicted as thick solid and dashed lines, respectively. The thin solid line is the \( \phi_{c}^{(A)}(X_0) \) glass transition line. The nematic instability occurs at \( \phi_{nem}(X_0) \) which is shown as thin dashed-dotted lines. The inset shows the situation around \( X_0 = 2.5 \) where the \( \phi_{c}^{(B)}(X_0) \) glass transition line merges into the \( \phi_{c}^{(B')}(X_0) \) transition line.

FIG. 2. The static structure factor \( S_{ll}(q,m) \) is plotted together with the non-ergodicity parameter \( F_{11}(q,m) \) for \( X_0 = 1.3 \) and \( \phi = 0.549 \) (directly above the non-ergodicity transition). Part a) shows the center of mass correlator \( l = l' = m = 0 \) whereas part b) shows the quadrupolar correlator \( l = l' = 2, m = 0 \).

FIG. 3. A similar plot as fig. 2 is shown but for \( X_0 = 2.3 \) and \( \phi = 0.617 \) (again directly above the non-ergodicity transition) which is already close to the nematic instability.

FIG. 4. At the glass transition the correlation length for parallel orientation obtained from the half-width of the peak of \( S_{ll}(q,0) \) is plotted as a function of the aspect ratio. For \( X_0 < 2.4 \) the glass transition is of type B whereas for \( X_0 > 2.5 \) it is of type B’ (see text).
FIG. 5. For $X_0 = 2.5$ and $\phi = 0.593$, the smallest aspect ratio where the type-B’ transition occurs first the $q$-dependence of the non-ergodicity parameter $F_{ll'}(q, m)$ is plotted together with the static structure factor $S_{ll'}(q, m)$ and the normalized non-ergodicity parameter $f_{ll'}(q, m) = F_{ll'}(q, m)/S_{ll'}(q, m)$. In (a) this is done for $l = l' = 2$ and $m = 0$ whereas (b) shows the same quantities for the center of mass $l = l' = m = 0$.

FIG. 6. The formation of the $\phi^{(B')}_{g}$ glass transition is illustrated. Within each domain of diameter $\xi$ the system shows liquid crystalline order whereas for $l \gg \xi$ there are randomly frozen orientational correlations.
$X_0 = 1.3$

Graph showing:

- $S_{00}(q,0)$
- $F_{00}(q,0)$
- $S_{22}(q,0)$
- $F_{22}(q,0)$
