Geometrical properties of the potential energy of the soft-sphere binary mixture

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We report a detailed study of the stationary points (zero-forces points) of the potential energy surface (PES) of a model structural glassformer. We compare stationary points found with two different algorithms (eigenvector following and square gradient minimization), and show that the mapping between instantaneous configuration and stationary points defined by those algorithms is as different as to strongly influence the instability index $K$ vs. temperature plot, which relevance in analyzing the liquid dynamics is thus questioned. On the other hand, the plot of $K$ vs. energy is much less sensitive to the algorithm employed, showing that the energy is the good variable to discuss geometric properties of the PES. We find new evidence of a geometric transition between a minima-dominated phase and a saddle-point-dominated one. We analyze the distances between instantaneous configurations and stationary points, and find that above the glass transition, the system is closer to saddle points than to minima.

I. INTRODUCTION

Interest in the geometric properties of the potential energy surface (PES) of liquids as a mean to understand their dynamics and thermodynamics dates back to the work of Goldstein [1] and Stillinger and Weber [2]. These works showed that to analyze the low temperature dynamics of supercooled liquids and glasses it is useful to map instantaneous configurations (ICs) to the (local) minimum of the PES found directly downhill, called inherent structure (IS). This mapping allows to disregard fast vibrations, focusing on slow, activated, structural relaxations. But if one aims to describe the dynamic crossover taking place around the the Mode Coupling theory (MCT) [3], the IS mapping is not useful because barriers between minima are no longer relevant at high temperatures and the two timescales cease to be well separated. Within the PES approach, two approaches have been proposed. One is to consider whole superstructures of minima (called metabasins [4–6]). Another is to focus on stationary points with some unstable directions: saddle points (SPs) [7].

The latter approach was motivated by results obtained on the $p$-spin model (a mean field glass model). In this system, a threshold energy exists which separates a low-energy, minima-dominated region, from a high-energy, saddle dominated one [8, 9]. The higher the energy, the larger the number $K$ of unstable directions of the typical SP (this number is called the order, or instability index of the SP, and is equal to the number of negative eigenvalues of the Hessian matrix evaluated at the SP). In this model the average index as a function of the energy $K(E)$ can be computed [8]. Furthermore, it can be verified directly that at high temperatures the stationary point closer to the typical IC is a SP with extensive $K$, while it is a minimum ($K = 0$) at low temperatures [10]. The dynamic arrest observed at the dynamic transition is related to the fact that the system starts getting trapped, or nearly trapped [11, 12]. A similar scenario was then proposed [7] for structural glasses: the glass transformation is the consequence of a geometrical transition. In the saddle-dominated (high energy) phase, the system can relax either by jumping an energy barrier or by finding an unstable direction. In the minima-dominated phase (low energy), the second mechanism is no longer available; as a consequence relaxation times soar. It was shown later that the two-step relaxation observed in the supercooled liquid (and described by Mode Coupling theory (MCT)) can be qualitatively understood as relaxation in the vicinity of a SP [13].

This scenario has been explored in several numerical studies of model liquids. Some of these works obtained estimations of the $K(E)$ curve [14–16], which have been found compatible with the existence of a geometric transition (further evidence for the transition has been found in the context of high frequency vibrations [17]). Other works have studied instead $K$ as a function of the temperature $T$ [18–22], showing that $K$ decreases dramatically on approaching $T_{MC}$. In early studies the view was held that a sharp transition can be observed as a function of temperature, with $K = 0$ for $T < T_{MC}$ and $K > 0$ for $T > T_{MC}$, but further work has shown [5, 21, 23] that although $K$ decreases very fast (most likely with an Arrhenius law [5, 24]), it is still nonzero for $T < T_{MC}$. This has prompted criticism of the saddle–minima transition point of view (see e.g. ref. 24), although a geometric transition, controled by the energy, is compatible with a smooth $K(T)$ curve (see sec. IV).

But there is another issue to be discussed when considering $K(T)$ curves. Since the system is never precisely at a SP, to define a $K(T)$ curve one needs to introduce a mapping between ICs and SPs (in a sense defining a

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“basin of attraction” of a SP, and generalizing the IS concept). Additionally, if one wants to somehow interpret dynamic behavior from such curve, the mapping should preserve at least some dynamic information. In analytical studies (e.g. [10, 25, 26]) ICs are (reasonably) mapped to the nearest SP (using the Euclidean distance or some overlap function). In contrast, in numerical work ICs are mapped to a SP through the algorithm used to find the latter, thus in principle introducing a dependence on the details of the procedure used to find SPs [25, 26] and raising the question of the dynamical relevance of the mapping. This is perhaps more worrying given that at least one popular procedure fails rather often, leaving some configurations unmapped (see ref. 21 and discussion below). Also puzzling are some results [21, 22] that seem to indicate that in the typical distance from an instantaneous configuration to a saddle or to a minimum is the same, at variance with the mean field situation.

In this paper we address the issue of the mapping between ICs and SPs, and analyze of distances between ICs and SPs and minima in more detail than has been previously done. Our results show that the $K$ vs. $T$ plots are algorithm-dependent, and that, at least in the soft-sphere model we consider, ICs at high temperature are closer to SPs with $K > 0$. The large number of SPs collected allows a new analysis which provides new evidence for the existence of a geometrical transition.

II. MODEL AND ALGORITHMS

We have considered the soft sphere binary mixture [27, 28], which consists of 50% of particles of type $A$ and 50% of type $B$, interacting with a pair potential $v_{ij}(r) = (\sigma_i + \sigma_j)^{12}/r^{12}$. The radii $\sigma_i$ are fixed by the conditions $\sigma_B/\sigma_A = 1.2$ and $(2\sigma_A)^3 + 2(\sigma_A + \sigma_B)^3 + (2\sigma_B)^3 = 4$. We have used a system of $N = 70$ particles at unit density and a smooth (cubic polynomial) long-range cut-off $\sqrt{3}$ as in ref. 16. We have used swap Monte Carlo [29] to equilibrate the system at temperatures $T = 1$, 0.683, 0.482, 0.350, 0.260, 0.220. For this system $T_{MC}$ is about 0.24 [16, 28]. At each temperature, 40000 equilibrated configurations were saved and used as starting point for minima and saddle point searches. Minima were obtained with Nocedal and Liu’s LBFGS algorithm [30], which code can be obtained from the internet [31]. For SP searches, two different algorithms were employed: square-gradient minimization (SGM) and eigenvector following (EF) (described below), to compare two different IC–SP mappings. In all, about $3.2 \cdot 10^5$ SPs were obtained.

A. Square gradient minimization

One way of finding SPs is minimizing the squared modulus of the gradient,

$$\phi = |\nabla V|^2 = \sum_{i=1}^{N} \sum_{\alpha=1}^{3} \left( \frac{\partial V}{\partial x_{i,\alpha}} \right)^2.$$  \hfill (1)

Since $\phi$ is nonnegative, at the absolute minima $\phi = 0$, which implies $\nabla V = 0$ (a saddle point). This method is relatively easy to implement, since good numerical minimization algorithms are publicly available (we have used LBFGS [30, 31]). The biggest drawback is that minimization can (and does rather often) converge to a local minimum, which is neither a saddle point, nor close to one in any reasonable sense [32].

B. Eigenvector following

This method has been specifically designed to find stationary points of the potential energy. Based on an original proposal by Cerjan and Miller [33], it has been substantially improved by others (see ref. 34 and references therein). The problem originally considered [33] was to find a saddle point of index 1 starting from a local minimum of $V$. The idea was to consider the function on a small sphere around the minimum. Using Lagrange multipliers and a quadratic approximation, one looks for local minima of the function constrained to the sphere. Close enough to the initial point (minimum), there is one local minimum of the constrained function that has higher energy: this is a point along the path that leads to the sought saddle point, and is taken as the starting point of the next iteration. Close to the saddle this criterion no longer applies, so a Newton-Raphson step is taken.

We have used our own implementation of the eigenvector following method as described by Wales and coworkers [22, 35–37]. At each iteration a step $\Delta x$ is proposed, which in the base that (locally) diagonalizes the Hessian is [35, 36]

$$\Delta x_{\mu} = S_{\mu} \frac{2g_{\mu}}{|h_{\mu}| \left( 1 + \frac{1}{1 + 4g_{\mu}^2/h_{\mu}^2} \right)},$$ \hfill (2)

where $h_{\mu}$ are the eigenvalues of the Hessian and $g_{\mu}$ are the components of the gradient in the diagonal base ($\Delta x_{\mu}$ is set to 0 for the directions where $h_{\mu} = 0$; i.e. uniform displacements). The sign $S_{\mu} = \pm 1$ is chosen as explained below. Note that as $g_{\mu} \rightarrow 0$,

$$\Delta x_{\mu} = -\frac{g_{\mu}}{h_{\mu}} + O(g_{\mu}^2), \quad g_{\mu} \rightarrow 0$$ \hfill (3)

where the first term is the Newton-Raphson step. A set of trust radii $\{\delta_{\mu}\}$ is maintained (one for each direction) [37]. The proposed step is rescaled so that $|\Delta x_{\mu}| \leq \delta_{\mu}$ for
all $\mu$, and then the position is updated. Initially, the $\delta_{\mu}$ are set to 0.2, and at each step are increased (decreased) by a factor 1.2 according to whether the quantity $r = (h_{\mu} - h_{\mu}'\delta_{\mu})$ is less (greater) than 1. $h_{\mu}$ is an estimation of the eigenvalue, $h_{\mu} = (g_{\mu} - g_{\mu}')/\Delta x_{\mu}'$, where the prime means the quantity evaluated at the previous iteration [37].

If $S_{\mu} = 1$, the step increases the energy along the direction $\mu$, thus the algorithm converges to a maximum along this direction. Conversely if $S_{\mu} = -1$ the algorithm converges to a minimum along $\mu$. Since a saddle point of order $K$ is a maximum along $K$ directions and a minimum along $3N - K$ directions, in principle the algorithm may be made to converge to a saddle of the desired index by setting $S_{\mu} = -1$ for $1 \leq \mu \leq K$, and $S_{\mu} = 1$ for $\mu > K$. In this work we do not want to fix the index from the start of the search, so for each starting configurations we run 20 steps with $S_{\mu} = -\text{sgn} h_{\mu}$ and only then fix the index to whatever value it has reached after the first 20 steps [22].

C. Distances

The distance we report is the Euclidean distance

$$d = \sqrt{\sum_{i,\alpha} (x_{i,\alpha} - y_{i,\alpha})^2},$$

minimized over the symmetry operations of the system (i.e. translations, the 48 discrete symmetries of the simple cubic lattice, and particle permutations). Minimization over translations is done applying Brent’s method [38, §10.2] to a distance minimized over the discrete symmetries and permutations. This in turn is found by exhaustive exploration of the discrete symmetries and using the Hungarian algorithm [39] (as implemented by B. Gerkey [40]) to minimize over permutations.

III. COMPARISON OF SGM AND EF MAPPINGS

A. Basins of attraction and success rate

In Fig. 1 where we show the rms gradient $g = \sqrt{\phi/N}$ of the configurations obtained after running SGM and EF on the same set of ICs. EF produces tightly converged saddle points ($g < 10^{-11}$), while the configurations found by SGM have rms gradients that cluster around about $10^{-6}$ and $10^{-2}$. To decide whether these configurations are saddle points and compute a success rate (Fig. 1, inset) we have used the SGM configurations as starting points for EF searches and computed the distance between the SGM and corresponding EF converged configurations. In some cases, after a few (3–5) steps, EF found a saddle very close to the SGM configuration (distances of the order of $10^{-5}$ to $10^{-2}$), while in other cases the distance was $O(1)$ or larger (and the number of steps increased). The first case clearly corresponds to an absolute minimum of $\phi$, and the second to a local minimum. The criterion we used to accept the SGM configuration as a true saddle was to require that the distance between it and the corresponding EF saddle be less than 0.01. This is approximately equivalent to requiring $g < 10^{-4}$ for the SGM configuration.

The high failure rate of the SGM algorithm makes it unsuitable to define basins of attraction of saddle points [21, 22]. This failure rate is not due to problems with the minimization algorithm, but to the high number of local minima of the function $\phi$ [14, 16, 21]. On the other hand the EF algorithm in principle will always converge to a saddle point (eventual failures being due to numerical problems or implementation details). However, it should be remembered that although basins of attraction for saddle points can be defined using EF, these are not necessarily a reasonable generalization of ISs. It is well known that iterative non-linear algorithms can lead to multiply connected or even fractal basins (a case of fractal basins is the Newton-Raphson algorithm applied to finding the roots of the polynomial $z^3 - 1$, see e.g. ref. 38, §9.4). In the case of EF, a detailed study on a 3-atom cluster [35] has shown that the basins, though not fractal, are still complex and multiply connected. Their relevance to liquid dynamics is thus not to be taken for granted. We have not performed such detailed analysis here, but in Fig. 2 we plot the instantaneous energy along a short (1000 steps) molecular dynamics (MD) run, along with the energy of the EF saddle points found starting from each IC. All these ICs map to a single IS (minimum). The strong energy fluctuations of the saddles found in

![FIG. 1: Root-mean-square gradient vs. energy of the configuration obtained with SGM or EF starting from 10000 equilibrium configurations at $T = 0.350$. Inset: success rate (fraction of initial configurations that converge to saddle points) vs. temperature (SGM: circles, EF: squares).](image-url)
FIG. 2: Instantaneous energy along a 1000-step MD run at $T = 0.260$ (dashed-dotted line) and energy of the saddle points found by EF using the MD configurations as starting points (full line). All instantaneous configurations correspond to a single IS.

this way indicate that the usefulness of the basins of attraction so defined is probably rather limited in understanding the liquid dynamics.

B. Saddle index curves

Let us first consider the saddle index vs. temperature curve. In Fig. 3 we plot separately the average value of $K$ for saddles obtained with EF and SGM. We also plot $K(T)$ evaluated for ICs (the eigenvectors of the Hessian evaluated at an IC are usually called instantaneous normal modes (INM)). The fact that the curves are algorithm-dependent prevents one from drawing any dynamical conclusion from them, unless there is some reason to expect that the mapping between ICs and SPs preserves some dynamical information. In particular, the critical temperature $T_0$ where $K(T_0) = 0$ (which might or might not be greater than zero) will be algorithm-dependent and thus not of much significance without further evidence of the dynamical relevance of the algorithm chosen to compute $K(T)$.

On the other hand, if we consider $K$ as a function of the energy of the saddle point (Fig. 3, right), the curves produced from the SPs collected with EF and SGM are essentially coincident in the region of energies where both algorithms find a significant number of saddles (see inset of Fig. 4). The corresponding curve for INMs (not shown) is very close to those corresponding to the SPs, in contrast to what is found in Lennard-Jones [14]. In this purely geometrical plot, the problem of the IC-SP mapping is avoided, and issues such as the existence of a geometrical transition can be meaningfully discussed.

Of course, this does not mean one should not worry about possible biases introduced by the algorithms. Indeed, if one considers the SPs within a given energy band, the distribution of the saddle index is slightly different, with EF tending to be slightly narrower (Fig. 4 shows a representative energy band). It is also clear that SGM tends to find SPs with lower energy (inset of Fig. 4). However, we find that the maximum of the log $N_{\text{samp}}$ vs. $K$ curves are the same for both algorithms at all energy bands. The significance of this maximum can be appreciated from the considerations of sec. IV.
C. Distances

Finally we consider the distances between ICs and the stationary points (IS, EF saddles and SGM saddles) obtained starting from the given IC. The distances reported here are those obtained after minimizing over the symmetries of the hamiltonian, as discussed in sec. II C. We have found that this distance coincides most of the time with the distance obtained without applying minimizations when one considers an IC and the stationary point obtained from it, so that the averages we report are not significantly different from those obtained without minimizing. Minimization is however important when computing distances between a configuration and a stationary point obtained from a different IC, as we do below.

The average distances as a function of temperature are plotted in Fig. 5. Two things are to be noted: first, SGM saddles are always closer than EF saddles; second, ISs are farther than SGM saddles at high temperatures but start to be found closer as temperature is lowered. The first fact points to the influence of the algorithm in defining an IC–SP mapping, stressing the problems of interpretation of $K(T)$ curves. The second provides direct evidence that at high temperatures there is a saddle point to be found closer to the typical IC than the corresponding IS.

To investigate this matter more closely, we look in detail at a short MD trajectory at $T = 0.26$, slightly above $T_{MC}$ (Fig. 6). For all ICs in this run, apart from computing the corresponding IS and SGM saddle as usual, we have searched for the nearest SP in the pool of all SPs found at the corresponding temperature. We find again that the system is mostly close to a saddle point of order $K \geq 1$, as can be also seen in the inset. This result is natural within the geometrical transition scenario, but

IV. SADDLE–MINIMA TRANSITION

Consider the number $N(K,E)$ of saddle points of order $K$ and energy between $E$ and $E + dE$. For short range interactions, one expects to be able to divide the system into effectively independent subsystems, so that $N(K,E)$ should be exponential in the size of the system $[22, 41]$. Then $\log N$ is extensive in the thermodynamic limit, and the complexity $\Sigma(k,e) = (1/N) \log N(K,E)$ is an intensive quantity. The (intensive) average saddle index can then be written ($e = E/N$)

$$\langle k(e) \rangle = \frac{1}{Z} \int_0^\infty \frac{K}{N} \exp[N\Sigma(K/N,e)] dK$$

(5)

and

$$= \frac{N}{Z} \int_0^\infty k \exp[N\Sigma(k,e)] dk,$$

(6)

where

$$Z = \int_0^\infty \exp[N\Sigma(k,e)] dk.$$

(7)

Using the saddle point method one gets

$$\langle k(e) \rangle = \tilde{k}(e) + O(1/N),$$

(8)
where $\hat{k}(\epsilon)$ is the point where $\Sigma(k, \epsilon)$ attains a maximum (with $\epsilon$ fixed), i.e. the solution of $\partial \Sigma(k, \epsilon)/\partial k = 0$. The saddle–minima transition should be understood as happening at the threshold energy $\epsilon_{th}$, defined as the maximum energy for which $\hat{k}(\epsilon) = 0$. In the thermodynamic limit this implies $\langle k(\epsilon \leq \epsilon_{th}) \rangle = 0$. In finite systems the average will remain positive, but the $\langle k(\epsilon) \rangle$ curve will show a fast crossover, remnant of the sharp $K$ band a histogram in opening at the threshold energy.

V. CONCLUSIONS

We have shown that in numerical studies of the PES of liquids, the algorithm chosen to associate instantaneous configurations and saddle points can have a significant influence in the analysis of quantities like the saddle index vs. temperature curve. Of the two algorithms used, we have found that the saddles found with SGM are closer to the instantaneous configurations than those found with EF. Since no such difference was found in ref. 22, the present results may reflect a property of the soft-sphere model, or of the present implementation of the EF algorithm. In any case, the point is that curves such as $K(T)$ are not meaningful unless the validity of the IC–SP mapping with respect to dynamic properties is established. It seems that neither of these algorithms is useful to define a partition of phase pase into basins of attraction of a SP (in the case of SGM it is rigorously impossible [21]).

The natural variable to analyze geometrical properties of the PES is the energy. We have shown that this choice of variable largely avoids the issue of the IC–SP mapping (in particular the $K(E)$ plot is mostly independent of the mapping), though the algorithms introduce some detectable bias in the sampling. We have produced an estimate of the shape of the saddle complexity that provides new evidence for the existence of a geometric transition in the soft-sphere model.

Finally, our analysis of distances has shown that in this model above $T_{MC}$ the system is closer to saddle points than to inherent structures, as has been shown to be the case in some mean-field models ($p$-spin [10], $k$-trigonometric [25]). We have also found that there are saddles closer than the SGM saddle (this has been explored analytically in the $k$-trigonometric model, where the SGM saddle was found to be the closest saddle [25], and the mean-field $\phi^4$ model, where it is not [26]).

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