Analysis of space correlations in a model 2D liquid through eigenvalues and eigenvectors of atomic level stress matrices

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Considerations of local atomic level stresses associated with each atom represent a particular approach to address structures of disordered materials at the atomic level. We studied structural correlations in a two-dimensional model liquid using molecular dynamics simulations in the following way: We diagonalized the atomic level stress tensors of every atom and investigated correlations between the eigenvalues and orientations of the eigenvectors of different atoms as a function of distance between them. It is demonstrated that the suggested approach can be used to characterize structural correlations in disordered materials. In particular, we found that changes in the stress correlation functions with decrease of temperature are the most pronounced for the pairs of atoms with separation distance that corresponds to the first minimum in the pair density function. We also show that angular dependencies of the stress correlations previously reported in [Phys. Rev. E 91, 032301 (2015)] are not related to the alleged properties of the stress field, but are a trivial consequence of the rotational properties of the stress tensor.

I. INTRODUCTION

It is relatively easy to describe structures of crystalline materials due to the presence of translational periodicity. This periodicity implies that atoms whose coordinates differ by a vector of translation have identical atomic environments. In glasses and liquids, in contrast, every atom, in principle, has a unique atomic environment \[2–6\]. For this reason description of disordered materials continues to be a challenge. Many different approaches have been suggested to describe disordered structures. However, none of them allows establishing a clear link between the structural and dynamic properties of disordered matter \[1, 2\].

The concept of local atomic level stresses was introduced to describe model structures of metallic glasses and their liquids \[2\]–\[6\]. For a particle \(i\) surrounded by particles \(j\), with which it interacts through pair potential \(U(r_{ij})\), the \(\alpha\beta\) component of the atomic level stress tensor on atom \(i\) is defined as \[3–6\]:

\[
\sigma_{\alpha\beta}^i = \frac{1}{V_i} \sum_{j \neq i} \left[ \frac{dU}{dr_{ij}} \right] \left( \frac{r_{ij}^\alpha r_{ij}^\beta}{r_{ij}} \right). \tag{1}
\]

The sum over \(j\) in \(1\) is over all particles with which particle \(i\) interacts. In \(1\) \(V_i\) is the local atomic volume. By convention, the definition without \(V_i\) corresponds to the local atomic level stress element \[7\]–\[8\]. Note that \(\alpha\)-component of the force acting on particle \(i\) from particle \(j\) is \(f_{ij}^\alpha = [dU(r_{ij})/dr_{ij}] (r_{ij}^\alpha/r_{ij})\), where \(r_{ij} = r_i - r_j\) is the radius vector from \(i\) to \(j\). Also note that the atomic level stress tensor \(1\) is symmetric with respect to the indexes \(\alpha\) and \(\beta\). Thus in 3D it has 6 independent components \[4\]–\[6\], while in 2D it has 3 independent components.

There are several important results associated with the concept of atomic level stresses. One result is the equipartition of the atomic level stress energies in liquids \[4\]–\[6\]. Thus the energies of the atomic level stress components were defined and it was demonstrated for the studied model liquid systems in 3D that the energy of every stress component is equal to \(k_bT/4\). Thus the total stress energy, which is the sum of the energies of all six components, is equal to \(6 \cdot k_bT/4 = (3/2)k_bT\), i.e., the potential energy of a classical 3D harmonic oscillator. An explanation for this result has been suggested \[4\]–\[6\]. The equipartition breaks down in the glass state. Then there was an attempt to describe glass transition and fragilities of liquids on the basis of atomic level stresses \[9\]. Another result is related to the Green-Kubo expression for viscosity. Thus the correlation function between the macroscopic stresses that enter into the Green-Kubo expression for viscosity was decomposed into the correlation functions between the atomic level stress elements. Considerations of the obtained atomic level correlation functions allowed demonstration of the relation between the propagation and dissipation of shear waves and viscosity. This result, after all, is not surprising in view of the existing generalized hydrodynamics and mode-coupling theories \[10\]–\[11\]. However, in Ref.\[7\]–\[8\]–\[12\] the issue has been addressed from a new perspective and the relation between viscosity and shear waves was demonstrated very explicitly.

Recently it has been claimed in Ref.\[14\] that considerations of the correlations between the atomic level stressess allow observation of angular dependence of the stress field which is present in liquids in the absence of any external shear. In many respects our attempt to understand the results presented in Ref.\[14\] lead to the present publication. Here we demonstrate that angular dependencies presented in Ref.\[14\] have nothing to do with any stress
FIG. 1. Atomic level stress tensor of any atom can be diagonalized. Obtained eigenvalues, \( \lambda_1 \) and \( \lambda_2 \), can be associated with the lengths of the principal ellipse’s axes. The orientation of the ellipse with respect to the reference coordinate system is given by the angle, \( \varphi \), between the longest ellipse’s axis and the \( x \)-axis of the reference frame.

field. Instead these angular dependencies trivially originate from the rotational properties of the stress tensors.

However, the ideas presented here go beyond the scope of Ref.[14]. Here we address the atomic level stresses and correlations between the atomic level stresses of atoms separated by some distance from a new and yet very natural perspective. It is surprising that this approach has not been investigated in detail before. Reasoning in a similar direction was presented in Ref.[15, 16]. However, considerations presented there do not address correlations between the atomic level stresses of different atoms.

The paper is organized as follows. In section II we present the idea of the approach. In section III we present expressions for certain stress correlation functions. In section IV we describe the results of our MD simulations. We conclude in section V.

II. STRESS TENSOR ELLIPSES

The atomic level stress tensor of atom \( i \) defined with equation (1) is real and symmetric. Thus it can be diagonalized. Thus in 2D two real eigenvalues (\( \lambda_1 \) and \( \lambda_2 \)) and two real eigenvectors of the stress tensor, \( \sigma_{ij}^{\alpha\beta} \), can be found. The tensor \( \sigma_{ij}^{\alpha\beta} \) in 2D has 3 independent components. It is clear that these 3 parameters determine 2 eigenvalues and the rotation angle that describes orientation of the orthogonal eigenvectors with respect to the reference coordinate system. Let us associate with each atom \( i \) an ellipse with principal axes oriented along the eigenvectors of \( \sigma_{ij}^{\alpha\beta} \) and having lengths \( \lambda_1 \) and \( \lambda_2 \), as depicted in Fig. 1.

Previously atomic level stresses were discussed mostly in 3D. In 3D symmetric atomic level stress tensors have 6 independent components. Thus, previously, in particular in discussions related to the atomic level stress energies, it was assumed that the local atomic environment of an atom is described by 6 independent stress components. However, in view of the present considerations, it is clear that if the atomic level stress tensor is diagonalized then its 3 eigenvalues describe the geometry of local atomic environment, while its 3 eigenvectors describe the orientation of the associated ellipsoid with respect to the chosen coordinate system.

In model metallic glasses in 3D atoms often have 12 or 13 nearest neighbours [1, 2, 17]. Working with atomic level stresses effectively reduces the richness of all possible local atomic geometries to just 3 numbers. Of course, that is more convenient than dealing with more numbers associated, for example, with the description based on Voronoi indexies [1, 2]. However, it is unclear for which purposes it is enough to consider only 3 numbers and for which purposes it may not be enough. In consideration of the stress correlations between two atoms in 3D there are 9 relevant parameters: 6 eigenvalues (3 on each atom) describe the geometries of the two ellipsoids and 3 parameters describe the orientation of one ellipsoid with respect to another.

In Ref.[15, 16] correlations between the eigenvalues of the same atom have been considered for 2D and 3D Lennard-Jones liquids. It was demonstrated that there are correlations between the eigenvalues of the same atom.

Here we are interested in the correlations between the stress elements of different atoms. If we want to consider stress correlations between two different atoms in 2D then we associate ellipses with both atoms and consider the correlations between the eigenvalues and the orientations of the ellipses, see Fig. 2. It is clear that in isotropic one component liquids all pair correlation functions should depend only on distance \( r_{ij} \).

In the orthogonal coordinate system based on the eigenvectors of a particular local atomic stress tensor this stress tensor, \( S' \), is diagonal with eigenvalues \( \lambda_1 \) and \( \lambda_2 \) on the diagonal. In potentials with repulsive and attractive parts the values of some \( \lambda \) can be negative. The negative value of \( \lambda \) corresponds to the case when the atomic environment of an atom is dilated along the eigenvector associated with this \( \lambda \). Here we assume that potentials
that we consider are purely repulsive. Such systems held together at some density by periodic boundary conditions. In such cases, both \( \lambda^1 \) and \( \lambda^2 \) are positive and we order them to have \( \lambda^1 \geq \lambda^2 \).

The local atomic level stress tensor, \( S_i \), of atom \( i \) in the reference coordinate system can be obtained from the stress tensor of atom \( i \) in the coordinate system of its eigenvectors, \( S'_i \), by rotation on angle \(-\varphi_i\). Tensor \( S'_i \) transforms under rotation according to \( S'_i = R(\varphi_i)S_i R^T(\varphi_i) \), where \( R(\varphi) \) is the 2D rotation matrix by angle \( \varphi \) (in positive or counterclockwise direction): \( R^{xx}(\varphi) = \cos(\varphi) \), \( R^{yy}(\varphi) = \sin(\varphi) \). Multiplication of the matrices leads to the following results:

\[
\sigma^{xx}_i = \lambda^1 \cos^2(\varphi_i) + \lambda^2 \sin^2(\varphi_i) ,
\sigma^{yy}_i = \lambda^1 \sin^2(\varphi_i) + \lambda^2 \cos^2(\varphi_i) ,
\sigma^{xy}_i = \sigma^{yx}_i = (\lambda^1 - \lambda^2) \cos(\varphi_i) \sin(\varphi_i) ,
\tan(\varphi_i) = \sigma^{xy}_i / (\lambda^1 - \sigma^{yy}_i).
\]

According to the last expression \( \varphi_i \in (-\pi/2, \pi/2) \). Physically angle \( \varphi_i \) is defined up to an integer multiple of \( \pi \) as rotation by angle \( \pi \) does not change the ellipse.

### III. Expressions for Selected Stress Correlation Functions

Our further goal is to demonstrate that various stress correlation functions between the stress elements of atoms \( i \) and \( j \) exhibit dependence on angle \( \theta_{ij} \). See Fig.2. We want to demonstrate that this dependence is not a consequence of the presence of any physical angular dependent stress field, as it is claimed in [14]. Instead, it is a consequence of the rotational properties of the stress tensor.

#### A. Stress correlation function \( \langle \sigma^{xy}_i \sigma^{xy}_j \rangle \)

From (4) the product of stresses on atoms \( i \) and \( j \) \( \sigma^{xy}_i \sigma^{xy}_j \) has the form:

\[
\sigma^{xy}_i \sigma^{xy}_j = (1/4)(\lambda^1 - \lambda^2)(\lambda^1 - \lambda^2) \sin(2\varphi_i) \sin(2\varphi_j).
\]

We then express angles \( \varphi_i \) and \( \varphi_j \) through the angles \( \psi_{ij} \), \( \psi_{ji} \), and \( \theta_{ij} \): \( \varphi_i = \psi_{ij} + \theta_{ij} \) and the same for \( j \) in (6). In this way we get:

\[
\langle \sigma^{xy}_i \sigma^{xy}_j \rangle = (1/8) \left[ \langle F_1 - F_2 \cos(4\theta_{ij}) \rangle + \langle F_3 \sin(4\theta_{ij}) \rangle \right],
\]

where

\[
F_1(r_{ij}) = \langle (\lambda^1 - \lambda^2)(\lambda^1 - \lambda^2) \cos(2\psi_{ij} - 2\psi_{ji}) \rangle, 
F_2(r_{ij}) = \langle (\lambda^1 - \lambda^2)(\lambda^1 - \lambda^2) \cos(2\psi_{ij} + 2\psi_{ji}) \rangle, 
F_3(r_{ij}) = \langle (\lambda^1 - \lambda^2)(\lambda^1 - \lambda^2) \sin(2\psi_{ij} + 2\psi_{ji}) \rangle.
\]

It is easy to see from (7) that \( \langle \sigma^{xy}_i \sigma^{xy}_j \rangle \) depends on \( \theta_{ij} \). Although a stress tensor as a whole does not depend on the choice of coordinates, its numerical representation in a particular basis (with \( \sigma^{xy} \) being a part of it) does. In principle, any physical quantity of interest can be written as an average of an expression which is invariant with respect to the change of coordinates. Pair correlation functions \( F_1, F_2, \) and \( F_3 \) in (8,9,10) provide an example of such quantities, i.e., they depend on the distance \( r_{ij} \), but not on the angle \( \theta_{ij} \).

Due to a mirror symmetry we must have \( F_3(r) = 0 \). This is because reflection with respect to the direction from \( i \) to \( j \) changes the signs of angles \( \psi_{ij} \) and \( \psi_{ji} \), but does not change the eigenvalues. In our simulations \( F_3 \) averages to zero up to the noise level.

In order to understand the meaning of correlation function \( F_1 \) let us consider the contribution from some atoms \( i \) and \( j \) to this function. It follows from (6) that:

1) If one of the ellipses is a circle, for example \( \lambda^1 = \lambda^2 \), then the contribution from this pair of atoms is zero. Thus correlation function \( F_1 \) contains contributions only from those pairs of atoms in which there are finite shear deformations of the environments of both atoms.
2) If ellipses of atoms \( i \) and \( j \) have the same orientation with respect to the line connecting them then \( \cos(2\psi_{ij} - 2\psi_{ji}) = 1 \) and the contribution from this pair of ellipses is the maximum possible contribution from the pairs of ellipses with the same distortions.
3) If ellipses of atoms \( i \) and \( j \) are orthogonal to each other, i.e., \( \psi_{ij} = \psi_{ji} \pm \pi/2 \) then \( \cos(2\psi_{ij} - 2\psi_{ji}) = -1 \) and the contribution from this pair is the minimum possible contribution.
4) If \( \psi_{ij} = \psi_{ji} \pm \pi/4 \) then the contribution is zero.

In order to understand the meaning of correlation function \( F_2 \) from (9) note the following:

1) As in the case with \( F_1 \), only pairs atoms in which both atoms have shear distortions contribute.
2) The maximum contribution, for given distortions, comes from the ellipses for which \( \psi_{ij} = -\psi_{ji} \), i.e., from those ellipses whose orientations are mirror-symmetric with respect to the line connecting them.
3) If the deviation from the mirror symmetry is \( \pi/2 \), i.e., \( \psi_{ij} = -\psi_{ji} \pm \pi/2 \) then the contribution is the minimum possible contribution.
4) If \( \psi_{ij} = -\psi_{ji} \pm \pi/4 \) then the contribution is zero.

Note also the following. If large axes of the ellipses of atoms \( i \) and \( j \) are aligned then these ellipses have the same orientation with respect to any line, not only the line that connects them. Thus it is likely that rather simple organization of ellipses provides a maximum to the function \( F_1 \). It is the organization when all ellipses have the same shear distortions and the same orientations. This observation might be of interest for understanding the nature of viscosity. It follows from the Green-Kubo expression that viscosity is determined by decay in time.
of the function $F_1$, i.e., for calculations of viscosity it is necessary consider stress of atom $i$ at time zero and stress of atom $j$ at time $t$ ($F_2$ does not contribute since integration over $\theta_{ij}$ in $F_1$ leads to zero).

B. Stress correlation function $\langle p_i \sigma_{jy}^{xy} \rangle$

Atomic level pressure on atom $i$ is defined as:

$$p_i = (\sigma_{ix}^{xx} + \sigma_{iy}^{yy})/2 = (\lambda_i^1 + \lambda_i^2)/2 .$$  (11)

Note that the trace of the stress tensor is invariant under rotation. From (11), similarly to how it was done for $\langle \sigma_{ix}^{yy} \sigma_{jy}^{xy} \rangle$, we get:

$$\langle p_i \sigma_{jy}^{xy} \rangle = (1/4) [F_4 \cos(2\theta_{ij}) + F_5 \sin(2\theta_{ij})] ,$$  (12)

where

$$F_4 = \langle (\lambda_i^1 + \lambda_i^2)(\lambda_j^1 - \lambda_j^2) \sin(2\psi_{ji}) \rangle ,$$  (13)

$$F_5 = \langle (\lambda_i^1 + \lambda_i^2)(\lambda_j^1 - \lambda_j^2) \cos(2\psi_{ji}) \rangle .$$  (14)

Again, due to a mirror symmetry, the function $F_4$ should (and it does in simulations) average to zero.

C. Stress correlation function $\langle (\sigma_{ix}^{xx} - \sigma_{iy}^{yy})\sigma_{jy}^{xy} \rangle$

For $\langle (\sigma_{ix}^{xx} - \sigma_{iy}^{yy})\sigma_{jy}^{xy} \rangle$ using (13,14) we write:

$$(1/2)(\lambda_i^1 - \lambda_i^2)(\lambda_j^1 - \lambda_j^2) \cos(2\varphi_i) \sin(2\varphi_j) .$$  (15)

This can be rewritten as:

$$(1/2)F_1 \sin(4\theta_{ij}) + F_6 \cos(4\theta_{ij}) ,$$  (16)
where \( F_1 \) is given by expression (8) and:

\[
F_6 = \langle (\lambda_1^1 - \lambda_2^1)(\lambda_1^2 - \lambda_2^2) \cos(2\psi_{ij}) \sin(2\psi_{ij}) \rangle ,
\]

(17)

It is easy to see that function \( F_6 \) should average to zero. We verified this in our simulations.

D. Simpler correlation functions and normalization of the correlation functions

Correlation functions \( F_{1,2,3,4,5,6} \) are somewhat complicated as they represent averaged products of three parameters. Before considering them it makes sense to consider simpler correlation functions which represent averaged products on two parameters only. It is reasonable to assume that stresses on particles which are far away from each other are not correlated. This makes it reasonable to consider the following correlation functions:

\[
G_{mm}(r_{ij}) = \left( \frac{1}{Z^2} \right) \langle (\lambda_1^1 - \lambda_2^1)(\lambda_1^2 - \lambda_2^2) \rangle - 1 ,
\]

(18)

\[
G_{mp}(r_{ij}) = \left( \frac{1}{Z^2} \right) \langle (\lambda_1^1 - \lambda_2^2)(\lambda_1^2 + \lambda_2^2) \rangle - 1 ,
\]

(19)

\[
G_{pp}(r_{ij}) = \left( \frac{1}{Z^2} \right) \langle (\lambda_1^1 + \lambda_2^2)(\lambda_1^2 + \lambda_2^2) \rangle - 1 ,
\]

(20)

\[
C_{2\pm}(r_{ij}) = \langle \cos(2\psi_{ij} \pm 2\psi_{ji}) \rangle ,
\]

(21)

IV. RESULTS OF MD SIMULATION

A. Stress correlation functions

In our Molecular Dynamics (MD) simulations we considered the same 2D system that has been studied in Ref. [14]. We used the same Yukawa potential and the same LAMMPS MD program [18, 19]. We also performed simulations on the system of the same size.

We prepared our system by melting triangular lattice at reduced temperature \( T = 5 \). After equilibration at \( T = 5 \) we gradually reduced temperature in several steps that followed by equilibration at every tem-
FIG. 6. (a) Atomic level stress correlation function $\langle \sigma^{xx}_i \sigma^{xy}_j \rangle$. See formula (7). The functions $F_1$ and $F_2$ in $\langle \sigma^{xx}_i \sigma^{xy}_j \rangle$ were normalized according to (22). The function $F_3$ is zero, besides the noise. It is clear that panel (a) of this figure is very similar to the panel (a) of Fig.5 in Ref.[14]. (b) Atomic level stress correlation function $\langle p_i \sigma^{xy}_j \rangle$. See formula (12). The function $F_4$ in $\langle p_i \sigma^{xy}_j \rangle$ averages to zero. Thus only function $F_5$ is left. In order to produce this figure we had to subtract the average pressure from the diagonal components of the atomic level stress tensor. Effectively this means that the value of $\lambda$ averaged over $\lambda^1$ and $\lambda^2$ of all atoms, i.e., $\lambda^{ave}$, was subtracted from the values of $\lambda^1$ and $\lambda^2$ of every atom. Because of this subtraction we can not use normalization (19) since $\langle \lambda^1 + \lambda^2 - 2 \lambda^{ave} \rangle$ averages to zero. Thus we used normalization (18) instead. We also scaled intensity on the z-axis by a factor of 4. It is obvious that panel (b) of this figure is very similar to the panel (b) of Fig.5 in Ref.[14]. (c) Atomic level stress correlation function $\langle (\sigma^{xx}_i - \sigma^{yy}_i)\sigma^{xy}_j \rangle$. See Eq.(16). Only function $F_1$ in $\langle (\sigma^{xx}_i - \sigma^{yy}_i)\sigma^{xy}_j \rangle$ is non-zero. We scaled the function by a factor of 10 along the z-intensity axis. It is clear that correlation function in panel (c) is rather similar to the correlation function in panel (c) of Fig.5 in Ref.[14]. There is a difference with the two “circles” at $r/a < 1$. It is possible that authors of Ref.[14] did not look into such small distances and thus in their figure these “circles” fall into the central green region. Besides this difference their figures and ours look rather similar.

temperature. An unimportant difference with the methodology presented in Ref.[13] is that after equilibration at every temperature we collected data in microcanonical (NVE) ensemble instead of the canonical (NVT) ensemble that was used in Ref.[14]. However, it is clear from the following results that this difference is not important for our purposes. Atomic configurations for the calculations of the correlation functions were collected at total energies which corresponded to the following temperatures: $T(3) = 3.06 \pm 0.04$, $T(2) = 1.97 \pm 0.03$, $T(1.4) = 1.43 \pm 0.02$, $T(1) = 0.99 \pm 0.02$. In our simulations, we reproduced the dependence of potential energy on temperature presented in Fig.1 of Ref.[14].

All correlation functions presented in this paper were obtained by averaging over 1000 configurations of $N = 2500$ particles. For temperature $T = 1$ the time interval between two consecutive configurations was $10^4$ MD steps. Each MD step corresponded to 0.001 of the time unit. During these $10^4$ MD steps the mean square atomic displacement reaches $\sim 1.38a^2$, where $a$ is the average interatomic distance.

Changes with temperature of different correlation functions per pair of particles are shown in Figs.3-4-5. The dependencies of the functions $F_1$, $F_2$ and $F_3$, i.e., all the non-zero ones, on distance are shown in Fig. 4. At $T = 1$ we have $Z_- = \langle \lambda^1 - \lambda^2 \rangle \approx 10.82$ and $Z_+ = \langle \lambda^1 + \lambda^2 \rangle \approx 40.48$.

Figures 3-4-5 demonstrate that there are $r_{ij}$-dependent correlations between the parameters of the atomic level stress ellipses and in their orientations. These correlations gradually decrease with increase of $r_{ij}$. It is clear that functions $G_{mn}(r)$ in Fig.3(a) and $\langle \sigma^{xy}_i \rangle$ in Fig.4(a) exhibit more pronounced changes than does PDF on decrease of temperature. It is also clear that the first peaks in $F_1$ and $F_2$ also demonstrate more pronounced changes on decrease of temperature than does PDF. However, it is also more difficult to interpret these changes. Yet, developing features in $\langle \sigma^{xy}_i \rangle$ suggest that some ordering happens in the mutual orientations of the ellipses associated with the atoms separated by the distance corresponding the first minimum of the PDF. There also appears to be a certain similarity in the behaviours of $\langle \sigma^{xy}_i \rangle$ and $\tilde{F}_1$. This similarity suggests that changes in $\tilde{F}_1$ are caused by changes in $\langle \cos(2\psi_{ij} - 2\psi_{ji}) \rangle$. See expressions (5) for $F_1$. Thus changes in $\tilde{F}_1$ are likely to be caused not by changes in the parameters of the stress ellipses, but by changes in the mutual orientations of the ellipses. However, also note that there are changes in $G_{mn}(r)$ in Fig.3(a).

Using formulas (7,2,16) it is easy to convert curves in Fig.5 into the 2D intensity plots shown in Fig.6(a,b,c). We did it for the curves corresponding to $T = 1$. It is obvious that these 2D plots are equivalent to those shown in Fig.5 of Ref.[14]. This demonstrates that the claim made in Ref.[14] concerning the presence of some angular dependent physical stress field in the studied equilibrium liquid is incorrect.
B. Is studied system a true liquid?

Finally, we comment on the following statement made in Ref.[14]. It is stated there that at $T = 1$ the system is in a true liquid state.

Let us say that two atoms are the nearest neighbours if they are separated by a distance smaller than the position of the first minimum in the PDF, i.e., $(r_{ij}/a) \leq 1.36$. We constructed the distribution of the angles $\theta_{ij}$ for the pairs of nearest neighbours averaged over various numbers of simulation frames. The probability distribution of $\theta_{ij}$ for a single frame is shown as the black curve in Fig.7. This figure suggests the presence of an underlying triangular lattice.

If the system were a true liquid then many atoms would have local environments rotated randomly with respect to each other and there would be no oscillations suggesting the presence of an underlying triangular lattice. The appearance of Fig.7 suggests that for the system to be in a liquid state we need either larger size ($N > 2500$) or higher temperature ($T > 1$).

V. CONCLUSION

It was demonstrated that it is possible to study liquid (and glass) structures through considerations of correlations between the eigenvalues and eigenvectors of the atomic level stress tensors on different atoms. It was shown that on decrease of temperature some of the relevant correlation functions exhibit pronounced changes which could not be guessed from the pair density function. Thus the suggested method provides additional information and it is of interest to investigate evolution of stress correlations with it in model supercooled liquids on decrease of temperature.

We also demonstrated that interpretations reported in Ref.[14] are essentially incorrect. In particular, authors of Ref.[14] claim that they observe some physical angular dependent stress field in an equilibrium liquid without external shear. We demonstrated that in order to observe “the angular dependent stress field” it is necessary to have atomic level stress correlations, i.e., functions $F_1$, $F_2$, and $F_3$ should be non-zero. However, the angular dependencies observed in Ref.[14] essentially originate from the transformational properties of the atomic level stress tensor under rotation. Thus angular dependencies observed in Ref.[14] are not related to the presence of any physical angular dependent stress field.

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