

Fluctuations in shear-jammed states: A statistical ensemble approach

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Abstract – Granular matter exists out of thermal equilibrium, *i.e.* it is athermal. While conventional equilibrium statistical mechanics is not useful for characterizing granular materials, the idea of constructing a statistical ensemble analogous to its equilibrium counterpart to describe static granular matter was proposed by Edwards and Oakshott more than two decades ago. Recent years have seen several implementations of this idea. One of these is the stress ensemble, which is based on properties of the force moment tensor, and applies to frictional and frictionless grains. We demonstrate the full utility of this statistical framework in shear-jammed (SJ) experimental states, a special class of granular solids created by pure shear, which is a strictly non-equilibrium protocol for creating solids. We demonstrate that the stress ensemble provides an excellent quantitative description of fluctuations in experimental SJ states. We show that the stress fluctuations are controlled by a single tensorial quantity: the angoricity of the system, which is a direct analog of the thermodynamic temperature. SJ states exhibit significant correlations in local stresses and are thus inherently different from density-driven, isotropically jammed (IJ) states.

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Introduction. – A remarkable property of systems in thermal equilibrium is that the probability of occurrence of a microscopic state is known a priori through the universal Boltzmann distribution $P_{\nu} = e^{-\beta E_{\nu}}/Z(\beta)$. Here, β is the inverse temperature and E_{ν} is the energy of the microstate The Boltzmann distribution defines characteristics ν. such as the relation between fluctuations and response [1]. By contrast, granular systems are intrinsically out of thermal equilibrium, and we lack a broad framework for describing their statistical properties [2]. The idea of constructing statistical ensembles to describe granular systems originated in a proposal by Edwards [3] that the fluctuations of slowly driven, dense granular systems was controlled by the ensemble of "blocked" states, granular assemblies in static, mechanical equilibrium. The original Edwards ensemble uses free volume in a granular system as the analog of energy in a Gibbsian statistical framework. A more recent model is the force network ensemble (FNE) [4,5], which has been useful in describing force fluctuations on fixed granular geometries. The stress

ensemble is a generalization of the original Edwards idea, and is based on a "conservation" principle that arises from the constraint of *local* force and torque balance on every grain [6]. Merging of the original Edwards ideas with the stress ensemble approach leads to an analog of the Boltzmann distribution for granular solids (blocked or jammed states), where the role of temperature is played by two distinct quantities: a) the compactivity which is conjugate to volume, and b) angoricity, a tensor that is conjugate to the force moment tensor of granular solids [7,8].

The applicability of the concept of angoricity as a temperature-like variable has been beautifully demonstrated in recent experiments using photoelastic disks [9]. In earlier work, the concept of angoricity was applied to analyze stress fluctuations in simulated assemblies of frictionless grains [7,10]. These granular solids, frictional assemblies in experiments, and frictionless in the simulations, shared the common feature that the solidification is density driven. They, therefore fall within the rubric of the universal jamming phase diagram [11], and can be viewed as zero-temperature limits of thermal, amorphous solids.

A class of granular solids that are far from equilibrium, and not described within the original jamming scenario are shear-jammed (SJ) states [12,13]. These solids are created through shearing without changing the density, which is a strictly non-equilibrium pathway for creating solids. They provide a unique opportunity for testing the stress ensemble with its full tensorial complexity in an ensemble that has no equilibrium analog. In this work we show that the stress fluctuations in SJ states are described quantitatively by the stress ensemble, which is the infinite compactivity limit of the generalized ensemble. This test of the stress ensemble is non-trivial since we demonstrate that stresses have non-trivial correlations in SJ states, unlike in density-driven granular solids.

The paper is organized as follows: The second section provides a brief review of experimental SJ states, the third section introduces the tensorial formulation of the stress ensemble framework, the fourth section presents results of testing the stress ensemble framework in SJ states, and finally, in the last section, we discuss the correlations in SJ states, and its implications.

Shear-jammed (SJ) states. – Dry grains interact with purely repulsive, contact interactions. Without any cohesion between them, the only way to create a solid of dry grains is by applying a load at the boundary. A common feature of most experimental [9,14] and numerical [15] techniques for creating jammed states is the application of isotropic pressure (we shall call these IJ states from here on). The jamming transition is defined as the onset of mechanical stability, and usually associated with a particular packing fraction, ϕ_J , [11] that can be protocol dependent. IJ states can also be sheared to study their response [15,16]. However, in these cases, shear stress should be considered a perturbation to an already jammed state, and under large enough shear stress, IJ states can unjam into flowing states.

In contrast, the observation of SJ states in experiments [12,13] and simulations [17] has demonstrated that applying isotropic pressure is not a necessary condition for jamming. For a range of packing fractions below the isotropic ϕ_J for a given protocol, jammed states can be created by applying shear only. The experimental SJ states, in two dimensions, are created through application of quasistatic, forward shear [12]. Packing fraction does not play a significant role in determining the properties of SJ states (fig. 1). For example, it has been shown that pressure and shear stress do not depend monotonically on ϕ as one would expect in IJ states, but rather monotonically scale with the fraction of force bearing grains in the system [12]. The SJ states are qualitatively different from IJ states. Whereas IJ states can have non-vanishing pressure and zero shear stress, pressure arises as a consequence of shearing in SJ states [13]. SJ states have strongly anisotropic fabric and force networks and stress tensors. It



Fig. 1: (Color online) Pressure vs. ϕ for all experimental states from [12]. Red: isotropic states with $\tau \approx 0$ (see also footnote¹). Blue: states with $\tau > 0$. States below the experimental pressure resolution, P_0 , cannot be identified for certain as jammed because of friction with base plate [12]. What is *certain* is that there are no isotropic states below ϕ_J , for these states there is a sharp transition to finite pressure at ϕ_J . For states with non-zero shear stress, there is no sharp transition as a function of the packing fraction.

has been shown that the SJ states emerge as a consequence of a percolation transition in the force network [12].

Stress ensemble. – Over a decade ago, Edwards and Oakeshott [3] theorized that the dynamics of slowly driven granular materials is controlled by the statistics of mechanically stable configurations, known as blocked A simple thermal system is specified by the states. state variables E, V, and N. In constructing a statistical ensemble for athermal granular materials, the role of the Hamiltonian in a thermal system is replaced by the volume function of a granular packing. Known as the Edwards ensemble, all blocked states of the same volume V are assumed to be equiprobable (microcanonical hypothesis). An entropy is defined for a granular state with the state variables V and number of grains N, S(V, N). The analog of the thermodynamic temperature can be defined by $X(V) = \partial V / \partial S$. X or the compactivity [3] is conjugate to the volume, and hence X = X(V) is also the primary equation of state. A microstate labelled by ν , inside a granular packing with total volume V is found with a probability proportional to the canonical distribution

$$P_{\nu} = \frac{1}{Z(X)} \exp[-w_{\nu}/X].$$
 (1)

Here, the volume function (analog of the energy E_{ν}) is determined by the set of grain positions $w_{\nu} = w(\{\vec{r}_i\})$.

The recent interest has focused on conservation laws and the sampling of the phase space of blocked states, especially in the context of extending the ensemble framework to stiff but not infinitely rigid grains. The basic aim of any ensemble approach is to predict the probability of

 $^{^1 \}rm The$ unjammed states (red points) at high pressure and low ϕ are actually isotropic states created by rare rearrangements of the anisotropic SJ states.

occurrence of a microscopic state, given a set of macroscopic, measurable quantities such as the volume and the external stress. A static granular packing is ultimately characterized by the positions of the grains, $\{\vec{r}_i\}$, and the set of contact forces, $\{\vec{f}_{ij}\}$. Specification of the forces is essential for defining static states of frictional grains, and it is therefore crucial to include the contact forces in a generalized statistical description for infinitely rigid and stiff grains. Among the various formulations there are two different ways to incorporate $\{\vec{f}_{ij}\}$ in an ensemble: 1) the FNE [6] in which micro states are characterized only by $\{\vec{f}_{ij}\}$, and 2) the stress ensemble [6–8]², which considers $\{\vec{r}_i\}$, and $\{\vec{f}_{ij}\}$. The latter, unlike the FNE, is not restricted to a fixed geometry.

In the stress ensemble, in addition to volume, granular blocked states are also characterized by the force moment tensor, which is a function of both grain positions $\{\vec{r}_{ij}\}$ and inter-granular forces $\{\vec{f}_{ij}\}$

$$\hat{\Sigma} = \sum_{i < j} \vec{r}_{ij} \otimes \vec{f}_{ij} \stackrel{2d}{=} \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{12} & \Sigma_{22} \end{pmatrix}.$$
 (2)

The constraint of local force balance leads to a conservation law for $\hat{\Sigma}$ [6,9], which states that the forcemoment tensor cannot be changed by local intervention such as tapping. Changing $\hat{\Sigma}$, while maintaining force balance on every grain, requires changing the forces on a line of grains that spans the system [6,7]. For a large system, there is thus a conservation principle reminiscent of energy conservation in non-dissipative systems. Taking tapping as an example for generating blocked states, the microcanonical stress ensemble is defined by fixing the values of V and $\hat{\Sigma}$. In addition to compactivity, the stress ensemble involves an intensive variable that is conjugate to $\hat{\Sigma}$. This is the angoricity tensor, $\hat{\alpha}^{-1}$, identified by Edwards and coworkers [3]. The relation between $\hat{\alpha}$ and $\hat{\Sigma}$ is analogous to the relationship between β and E in a thermodynamic system.

In a canonical ensemble formulation [7], the probability of obtaining a microstate ν with volume w_{ν} and force moment tensor $\hat{\Sigma}_{\nu}$ is given by a *tensorial* generalization of the Boltzmann distribution

$$P_{\nu} = \frac{1}{Z(X,\hat{\alpha})} \exp\left(-\frac{w_{\nu}}{X}\right) \exp\left(-\hat{\alpha}:\hat{\Sigma}_{\nu}\right), \quad (3)$$

where ":" stands for tensor contraction and the angoricity tensor $\hat{\alpha}^{-1}$ is defined by

$$\alpha_{kl} = \frac{\partial S(V, \Sigma)}{\partial \Sigma_{kl}} \bigg|_{V}.$$
(4)

In two dimensions, we have

$$\hat{\alpha} = \begin{pmatrix} \alpha_{11} & \alpha_{12} \\ \alpha_{12} & \alpha_{22} \end{pmatrix}.$$
 (5)

In the above thermodynamic formulation, the entropy $S(V, \hat{\Sigma})$ should be taken as the large M limit of the entropy of M-grains. Since all blocked states are in force and torque balance, their force moment tensor $\hat{\Sigma}$ is always symmetric, hence $\hat{\alpha}$ is also symmetric via eq. (4). It should be noted that while both $\hat{\alpha}$ and $\hat{\Sigma}$ transform like tensors under rotation, the argument of the Boltzmann term in eq. (3) contains only terms that are rotationally invariant scalars, which, as analog of βE , it should be. Also as a result the entropy can only depend on rotational invariants of the force moment tensor, *i.e.* $S(V, \hat{\Sigma}) =$ $S(V, \text{tr}(\hat{\Sigma}), \det(\hat{\Sigma})).$

Volume fluctuations in SJ states are less relevant than they are in IJ states. Analysis of SJ states shows that stress fluctuations and volume fluctuations are decoupled, and unlike IJ states, the packing fraction is not a state variable that determines the jamming probability under the shearing protocol [12]. These observations suggest that the pure stress ensemble, obtained in the limit of $X \to \infty$ is the one relevant for describing the fluctuations of SJ states. For a subset m < M of the particles, the pure stress ensemble [7] is defined by the canonical distribution

$$P(\hat{\Sigma}_m) = \frac{1}{Z(\hat{\alpha})} \exp\left[S_m(\hat{\Sigma}_m)\right] \exp\left(-\hat{\alpha}:\hat{\Sigma}_m\right).$$
 (6)

The canonical distribution (eq. (6)) describes the stress fluctuation in a region containing the *m*-grains that is in a "angoricity" bath due to the remainder of the system (see fig. 2(a)). $S_m(\hat{\Sigma}_m)$ is the (microcanonical) entropy function which is defined by counting the number of microstates

$$S_m(\hat{\Sigma}_m) \propto \log\left[\sum_{\nu} \omega_{\nu} \ \delta(\hat{\Sigma}_m - \hat{\Sigma}_{\nu})\right].$$
 (7)

In this formulation, we have allowed for the possibility of microstates not being sampled equally by including a microscopic weight ω_{ν} for state ν [18]. The stress ensemble and the original Edwards ensemble has be extended to include this possibility [6,19].

Measuring angoricity. – In order to apply eq. (6) to the experimentally generated SJ states, we need a measure of $\hat{\alpha}$. Unfortunately, we have no "thermometer" for directly measuring angoricity, and have to base its measurement on postulated or measured equations of state relating $\hat{\alpha}$ to $\hat{\Sigma}$.

In IJ states, a scalar version of eq. (6) is applicable, and there is a scalar α that is conjugate to Γ , the trace of the force moment tensor. In [10], the stress ensemble was applied to analyze pressure fluctuations in simulated frictionless IJ states, and an equation of state was deduced from these measurements. More recently, an equation of state has been deduced from measurements in IJ states of frictional packings [9]. In both systems, a linear relation was found between the inverse angoricity and Γ_M of an Mgrain system: $\alpha \approx \frac{M}{\Gamma_M}$. Since this linear relation worked

 $^{^{2}}$ We emphasize that the stress ensemble described here is not on a fixed geometry, but rather it comprises of states with different contact and force networks.



Fig. 2: (Color online) (a) Schematic demonstration of a subregion of size m and $\hat{\Sigma}_m$ inside a packing with $(M, \hat{\Sigma}_M)$. Here we define subregions as any contiguous cluster of m-grains roughly circular in shape. (b) Equation (6) predicts that when the distribution of local force moment tensor is multiplied by $e^{\hat{\alpha}:\hat{\Sigma}}$ (shown in the inset for m = 15 and the 22-component of the local force moment tensor in SJ states), its logarithm should be related to the entropy of microstates S_m , and for different $\hat{\alpha}'s$ this function should only differ by an additive constant. After a shift of each curve by Z_{22} calculated from the eq. (12), we find that the data collapse onto a universal curve in the main figure. The functional form of the collapses data also shows good agreement with the postulated form of entropy (eq. (13)), given by the solid red line.

quite well for pressure fluctuation in IJ states, we take a straightforward generalization of this as a postulate for the equation of state for SJ states.

$$\hat{\alpha} \propto M \left(\hat{\Sigma}_M \right)^{-1} = \frac{M}{\det \left(\hat{\Sigma}_M \right)} \begin{pmatrix} \Sigma_{22,M} & -\Sigma_{12,M} \\ -\Sigma_{12,M} & \Sigma_{11,M} \end{pmatrix}.$$
 (8)

Using this equation of state, each *M*-grain SJ state can be labelled by an angoricity tensor, since the force moment tensor is measured in the experiments. In the experiments, $M \sim 1000$, and one could wonder about this being large enough to be in the thermodynamic limit. We will address this question below through analysis of the convergence of the entropy function.

Equation (6) predicts the distribution of stress in a subregion containing m-grains at the angoricity given by $\hat{\alpha}$. As has been pointed out before [19], this Boltzmannlike distribution has a very special form. It has a term that depends purely on $\hat{\Sigma}$, a term that depends purely on $\hat{\alpha}$, and the combination of these two variables appears only in the exponential. The stress ensemble would, therefore, predict that multiplying the distribution by $e^{\hat{\alpha}:\hat{\Sigma}}$ and taking its logarithm would yield a function that depends on $\hat{\Sigma}$ and distributions corresponding to different $\hat{\alpha}s$ would differ only by an additive constant, or

$$\log\left[P(\hat{\Sigma}_m)e^{\hat{\alpha}:\hat{\Sigma}_m}\right] = S_m\left(\hat{\Sigma}_m\right) - \log Z(\hat{\alpha}).$$
(9)

We directly test these predictions as follows. All SJ states, regardless of the value of the shear strain or the packing fraction ϕ , are categorized by their global force moment tensor $\hat{\Sigma}_M$. Through the equation of tensor component Σ_{kl} can be obtained from eq. (6) and

state (eq. (8)), the value of the angoricity tensor is determined. Then for each SJ state at a particular $\hat{\alpha}$, random contiguous clusters containing m-grains (fig. 2(a)) are chosen to form an ensemble of subregions with different values of $\hat{\Sigma}_m$, giving a probability distribution $P_{\hat{\alpha}}(\hat{\Sigma}_m)$. To simplify the analysis, we avoid dealing with the multidimensional distribution function and instead, we analyze the reduced distributions for each component of the local force moment tensor.

Figure 2(b) shows that the data collapse implied by eq. (9) works remarkably well for a subregion containing 15 grains. We find similar data collapse for the other components of the force moment tensor, and for m as small as 4. For smaller m, there is more of a spread in the data, however, there is remarkably fast convergence as a function of m to a universal functional form, which we can interpret as the thermodynamic entropy $S(\Sigma_{kl})$ for kl = 11, 22, 12. The solid red line in fig. 2(b) is the functional form deduced from the assumed equation of state and the definition of $\hat{\alpha}$ (eq. (4))

$$S_M(\hat{\Sigma}_M) = A \ M \ \log \left| \det \ \hat{\Sigma}_M \right| \,. \tag{10}$$

Here, A = 0.5 is a constant of proportionality that is determined from the best fit to the collapsed data. A few features of fig. 2(b) are of note: there is a small but systematic difference between the entropy deduced from the equation of state, and the form of the collapsed data, especially at small values of Σ_{kl} . In spite of these small differences, the fact that we can collapse the data demonstrates that the Boltzmann-like distribution defined by an angoricity tensor (eq. (6)) works remarkably well for SJ states.

The equation of state that we postulated is the analog of an ideal-gas equation of state relating temperature and energy. If the entropy implied by this equation of state (eq. (10)) were to hold exactly for the SJ states, then it would imply that stress correlations in these states are shorter-ranged than the size of the m-grain subregions that we have analyzed. Below, we assume that the ideal-gas entropy holds, deduce an explicit scaling form for the distribution of stresses for m-grain subregions, and show that the ideal-gas model fails to describe the distributions in detail, and especially their scaling with m. To understand this observation, we analyze the variance of the components of the stress, and what it implies for stress correlations. Finally, we discuss how to reconcile the success of the equation of state with these observations.

Since the SJ states are created with bi-axial shear the resulting normal stress $\Sigma_{11,M} - \Sigma_{22,M}$ is much larger $(\sim 10 \text{ times } [12])$ compared to the off-diagonal component $\Sigma_{12,M}$. This justifies expanding the equation of state, eq. (8) to first order in

$$\frac{(\Sigma_{12,M})^2}{\Sigma_{11,M} \ \Sigma_{22,M}} \ll 1.$$
(11)

Then, reduced distributions of a particular force moment



Fig. 3: (Color online) (a) Probability distributions for the reduced variable defined in eq. (14). Solid red curves are theoretical predictions (eq. (15) with fitting parameter A = 1/2). m indicates number of grains in the subregion over which the local force moment tensor is defined. (b) Probability distributions for the reduced variable defined in eq. (16). Solid red curves are theoretical predictions. m indicates number of grains in the subregion over which the local force moment tensor is defined.

eq. (10) by integrating out all other components $mn \neq kl$. For the 11 and 22 components

$$p_{11,m}(\Sigma_{11,m}) \equiv \int d\Sigma_{22} \, d\Sigma_{12} \, P(\hat{\Sigma}_m) = \frac{\alpha_{11}^{m/2+3/2}}{\Gamma(m/2+3/2)} e^{S_{red}(\Sigma_{11,m})} e^{-\alpha_{11}\Sigma_{11,m}};$$
(12)

$$p_{22,m}(\Sigma_{22,m}) \equiv \int d\Sigma_{11} d\Sigma_{12} P(\tilde{\Sigma}_m) = \frac{\alpha_{22}^{m/2+3/2}}{\Gamma(m/2+3/2)} e^{S_{red}(\Sigma_{22,m})} e^{-\alpha_{22}\Sigma_{22,m}};$$

where we have introduced a reduced version of the entropy (eq. (10)) that depends on one force moment tensor component only

$$S_{red}(\Sigma_{11,m}) = (\Sigma_{11,m})^{(m/2+1/2)};$$

$$S_{red}(\Sigma_{22,m}) = (\Sigma_{11,m})^{(m/2+1/2)}.$$
(13)

This form of the distribution for $\Sigma_{11,m}$ and $\Sigma_{22,m}$ at various $\hat{\alpha}$'s can be collapsed by defining the rescaled

dimensionless variables

$$x = \frac{1}{m} \alpha_{11} \Sigma_{11,m}, \text{ or}$$

$$x = \frac{1}{m} \alpha_{22} \Sigma_{22,m},$$
(14)

yielding a gamma distribution

$$g_m(x) = \frac{m/2 + 3/2}{(m/2)^{m/2 + 3/2}} x^{m/2 + 1/2} e^{-mx}.$$
 (15)

The rescaled distributions from SJ states are compared to the prediction eq. (15) in fig. 3(a) for various local subregion sizes ranging from m = 5 to 71. This comparison shows that the theoretical prediction captures the mean and overall shape of the experimental distributions, but that theory and experiment differ significantly in the width of the distributions.

There is no simple scaled form for the off-diagonal component $\Sigma_{12,m}$, but in the limit of eq. (11) or $\alpha_{12} \rightarrow 0$, we can write a reduced distribution of $\Sigma_{12,m}$ in terms of rescaled local force moment components

$$x = \sum_{12,m} / \sqrt{\sum_{11,m} \sum_{22,m}}$$
 (16)

to obtain

$$h_m(x) = \frac{\Gamma(m/2 + 3/2)}{\Gamma(m/2 + 1)} \left(1 - x^2\right)^{m/2}.$$
 (17)

In fig. 3(b), we plot eq. (17) for several *m*-values compared with SJ data. In this case, there is very good agreement between theory and experiment, including the variance.

Discussion. - Figure 3(a) clearly shows that the variance of the local force moment tensor $\hat{\Sigma}$ is not well described by an ideal-gas-type model, particularly for small m. To explore this deviation further, we studied the scaling of the variance with the number of grains, m. As shown in fig. 4, the variances of all components of the stress scale as m^{γ} , with $\gamma \approx 1.5$. We note that the variance is related to the integral of the two-point, spatial correlation function of the force moment tensor of grains. The observed scaling, with an exponent larger than unity, can only arise if the correlations are long-ranged and do not decay within the region containing m-grains [20]. Since our scaling is valid for $m \approx 100$, which corresponds approximately to a 10×10 grain subregion, we can deduce that stress correlations do not decay away by 10 neighbors. The observed scaling of the variance of stress components in the SJ states is in sharp contrast to the experimental observation in IJ states, where the variance scales as m [9]. Interestingly, the variance of the scaled stress defined in eq. (16) scales as m indicating that this scaled stress does not have long-range correlations. For both IJ and SJ states, there is a well defined thermodynamic limit. SJ states converge with $\sqrt{\langle (\delta \Sigma)^2 \rangle} / \langle \Sigma \rangle \sim m^{-0.25}$, while IJ states converge faster with $\sqrt{\langle (\delta \Sigma)^2 \rangle} / \langle \Sigma \rangle \sim m^{-0.5}$.



Fig. 4: (Color-online) log-log plot of the variances for each local force moment tensor component as function of m. The variances are scaled by arbitrary stress scales to make them dimensionless. Dotted lines indicate the trend of $m^{1.5}$.

Since the probability of occurrence of SJ states is welldescribed by the Boltzmann-like distribution of eq. (6), we can use our experience with equilibrium statistical mechanics calculations to reconcile the ability of the idealgas framework to describe the equation of state with the presence of long-range correlations. It is known [20] that two-point correlations enter calculations of entropy (or free energy) through logarithmic corrections. It is, therefore, reasonable to expect that the entropy and the equation of state are much less sensitive to the existence of correlations than the variance of the force moment tensor. The longranged correlations in the local force moment tensor are indicative of long force chains that are clearly visible in SJ states [12,21]. We are currently investigating the microscopic origin of the observed long-range correlations.

In this work, we have demonstrated that the stress ensemble provides an excellent quantitative description of fluctuations in experimental SJ states. We show that the stress fluctuations are controlled by a single tensorial quantity —the angoricity of the system, which is a direct analog of the thermodynamic temperature. We show that the SJ states exhibit significant correlations in local stresses in sharp contrast to IJ states. This observation reinforces the conclusion [12] that SJ states are not merely density-driven jammed states created at a lower density. These states are inherently different from density-driven IJ states.

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