Euclidean random matrices, the glass transition and the Boson peak

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In this paper I will describe some results that have been recently obtained in the study of random Euclidean matrices, i.e. matrices that are functions of random points in Euclidean space. In the case of translation invariant matrices one generically finds a phase transition between a phonon phase and a saddle phase. If we apply these considerations to the study of the Hessian of the Hamiltonian of the particles of a fluid, we find that this phonon-saddle transition corresponds to the dynamical phase transition in glasses, that has been studied in the framework of the mode coupling approximation. The Boson peak observed in glasses at low temperature is a remanent of this transition.

I. INTRODUCTION

In the last years many people have worked on the problem of computing the properties of Euclidean random matrices. The problem can be formulated as follows. We consider a set of N points \((x_i)\) that are randomly distributed with some given distribution (two extreme examples are: a) the \(x\)’s are random independent points, b) the \(x\)’s are one of the many minima of a given Hamiltonian).

In the simplest formulation, given a function \(h(x)\), we consider the \(N \times N\) matrix:

\[
M_{i,k} = h(x_i - x_k) .
\]

The problems consists in computing the properties of the eigenvalues and of the eigenvectors of \(M\). Of course, for finite \(N\) they will depend on the instance of the problem (i.e. the actually choice of the \(x\)’s), however system to system fluctuations for the intensive quantities (e.g. the spectral density \(\rho(z)\)) disappear when we consider the limit \(N \to \infty\) at fixed particle density.

The problem is not new; it has been carefully studied in the case where the positions of the particles are restricted to be on the lattice. The case where the particles can stay in arbitrary positions, that is relevant in the study of fluids, has been less studied, although in the past many papers have been written on the argument [1]. These off-lattice models present some technical (and also physical) differences with on-lattice models.

A certain number of variations are interesting. For example we could consider the case where we add a term on the diagonal:

\[
M_{i,k} = \delta_{i,k} \sum_j h(x_i - x_j) - h(x_i - x_k) .
\]

In this case the associated quadratic form is given by

\[
\sum_{i,k} \phi_i \phi_k M_{i,k} = \frac{1}{2} \sum_{i,k} h(x_i - x_k)(\phi_i - \phi_k)^2
\]

and therefore the matrix \(M\) is non-negative if the function \(h\) is non-negative. The matrix \(M\) has always a zero eigenvalue as consequence of the invariance of the quadratic form under the symmetry \(\phi_i \to \phi_i + \lambda\); the presence of this symmetry has deep consequences on the properties of the spectrum of \(M\) and, as we shall see later, phonons are present.

In the same spirit we can consider a two-body potential \(V(x)\) and introduce the Hamiltonian

\[
H[x] = \frac{1}{2} \sum_{i,k} V(x_i - x_k) .
\]

We can consider the \(3N \times 3N\) Hessian matrix
\[ M_{i,k} = \delta_{i,k} \sum_j V''(x_i - x_j) - V''(x_i - x_k) . \] (5)

where for simplicity we have not indicated space indices. Also here we are interested in the computation of the spectrum of \( M \). The translational invariance of the Hamiltonian implies that the associated quadratic form is invariant under the symmetry \( \phi_i \to \phi_i + \lambda \) and a phonon-like behaviour may be expected.

This tensorial case, especially when the distribution of the \( x \)'s is related to the potential \( V \), is the most interesting from the physical point of view (especially for its relations to the theory of fluids), however it is technically more involved, so that it may be convenient to study in details the previous scalar cases in order to improve our command of the tools that are needed in the computations.

Our aim is to get both a qualitative understanding of the main properties of the spectrum and of the eigenvalues and a quantitate, as accurate as possible, analytic evaluation of these properties. Quantitative accurate results are also needed because the computation of the spectral density is a crucial step in the microscopic computation of the thermodynamic dynamic properties of glass forming systems. In some sense this approach can be considered as an alternative route to obtain mode-coupling like result, the main difference being that in the mode coupling one uses a coarse grained approach and the hydrodynamical equations, while here we take a fully microscopic point of view.

Before describing the progresses that have been done in the field I will recall some of the physical interesting cases for which this approach may be useful. This will done in the next two sections.

### II. GLASSES AT LOW TEMPERATURE

Let us consider a potential \( V \) such that the system forms a glass at low temperature. In this situation the Hamiltonian \( H \) has an exponential large number of minima i.e. proportional to \( \exp(aN) \) where \( a \) is a number of order 1. We can consider two different cases: (a) the variables \( x \) are at the absolute minimum of \( H \), (b) the variables \( x \) belong to a generic minimum of energy density \( E \).

In the real world, if we cool a glass at very low temperatures, it will not evolve toward the absolute minimum, characterized by an energy density \( E_0 \), but it will evolve toward local minima that have an higher energy density \( E \), depending on the details of the history of the sample; these minima are usually called inherent structures. In both cases, at low temperature the dynamics and the thermodynamics will be dominated by small harmonic vibrations around the minimum, i.e. the ISNM (inherent structure normal modes).

Qualitatively the spectrum of these vibrations is well known. No negative eigenvalues are present; at very low energy we have the phonons, at higher energy we have the famous Boson peak (the Boson peak is defined as a bump at some small but non-zero value of the eigenvalue \( z \) of the spectral density \( \rho(z) \) divided \( z^2 \)), \(^1\) whose origine will be discussed later in details, at still higher energy we have the main component of the spectrum and at very high energy there is the tail of localized states. The presence of some localized states in the low energy region is still matter of debate. The fact that the sound velocity is approximatively constant in the region of the Boson peak was considered amazing.

There are many other quantities that we would like to compute, in particular the structure function \( S(z, k) \) that can be directly experimentally measured. Moreover the width of the acoustic peak \( \Gamma(z) \) has an interesting behaviour at low \( z \) that is related to the behaviour of sound attenuation as function of the frequency.

In the long run we are also interested to understand quantum effects. There are trivial quantum effects that are related to the form of the spectral density; there are also more interesting quantum effects, e.g. two levels systems, that cannot be explained in the small fluctuation limit. However it is quite plausible the a good control of the quadratic part of the potential may be useful in getting quantitative predictions on these non linear effects.

\(^1\)The ratio \( \rho(z)/z^{1/2} \) usually go to a constant at \( z = 0 \), if we consider the the spectrum of the vibrations of a solid; at low value of the eigenvalue \( z \) the vibrations are phonons.
III. THE DYNAMICAL GLASS TRANSITION

A. The mean field scenario

It is usually believed that in the real world fragile glasses have only one transition with divergent viscosity (at temperature $T_K$). This transition cannot be observed directly because the time required for thermalization is too long. This transition is believed to be related to Kauzmann entropy crisis and it should happens just at the point where the configurational entropy becomes zero. The viscosity is supposed to diverge $\exp(A/(T - T_K))$ and the specific heat should be discontinuous.

However in the idealized world of mean field theories (e.g. the mode coupling theory or the equivalent replica approach), where activated processes are strictly forbidden, there is a second purely dynamics transition $T_c$ at higher temperatures [2]. Here the viscosity is divergent as a power law of $T - T_c$. This idealization is not so bad in the real world: activated processes are strongly depressed and the viscosity may increase of many order of magnitude (e.g. 6) before reaching the region where activated processes become dominant.

As it happens in many cases, slow relaxation is related to the existence of zero energy modes and this statement is true also in the mode coupling theory. This statement can be easily verified in spin models where the mode coupling theory is exact and simple computations are possible.

\[
\text{FIG. 1. The qualitative behaviour of the spectrum in mean field approximation above } T_c, \text{ (full line), at } T_c \text{ (dot-dashed line) and below } T_c \text{ (dashed line) as function of the eigenvalue } \lambda. \]

The general idea is quite simple. Let us consider the free energy as functional of the density $\rho(x)$ (i.e. $\mathcal{F}[\rho]$) (in a magnetic system the free energy as function of all the local magnetizations). We expect that at $T > T_c$ the only relevant solution for the thermodynamics is the trivial solution $\rho(x) = \text{const}$. At low temperatures there are an exponential large number of non-equivalent solutions where the the density has a non trivial dependence on $x$. Skipping many details the situation is the following:

- A temperature $T > T_c$ there are no non-trivial relevant solutions of the equation

\[
\frac{\delta F}{\delta \rho(x)} = 0, \tag{6}
\]

however the dynamics is dominated by quasi solutions of the previous equations, i.e. by densities $\rho(x)$ such that the left hand side of the previous equation is not zero, but vanishes when $T$ approach $T_c$. These quasi solutions are relevant for the dynamics [4]. One can compute the spectrum of the Hessian.
\[ M(x, y) = \frac{\delta^2 F}{\delta \rho(x) \delta \rho(y)}. \] (7)

One finds that \( M \) has negative eigenvalues and its spectrum extends to the negative eigenvalue region and has qualitatively the shape shown in fig. 1. These quasi stationary points of \( F \) look like saddles.

- At the transition point \( T = T_c \) the quasi stationary points becomes real solutions of the equations (6). They are essentially minima: the spectrum of the Hessian is non-negative and it arrives up to zero. As it can be checked directly, the existence of these nearly zero energy modes is responsible of the slowing down of the dynamics. The different minima are connected by flat regions so that the system may travel from one minimum to an other [3].

- At low temperature the mimima become more deep, the spectrum develops a gap as shown in fig. 1 and the minima are no more connected by flat regions. If activated processes were suppressed, the system would remains forever in one of these minima. In the real world the system may jump (by decreasing his energy) until it reaches the region where the minima are so deep that the energy barriers among them diverges.

This picture is not so intuitive because it involves the presence of saddles with many directions in which the curvature is negative, and it is practically impossible to visualize it by making a drawing in a two or a three dimensional space.

This qualitative description can be easily verified in models where the mean field approximation is exact. In glass forming liquid, the picture is essentially sound (provided that we correct it by considering the existence of phonons). However, if we try to test it a more precise way, we face the difficulty that the free energy functional \( F[\rho] \) is a mythological object whose exact form is not exactly known and consequently the eigenvalues of its Hessian cannot be computed. We will see in the next two subsections that the so called instantaneous normal modes (INM) are a first approximation to the eigenvalues of the Hessian of \( F \) and that a more interesting realization is provided by the saddle normal modes (SNM).

### B. Instantaneous normal modes

Instantaneous normal modes in liquid and glasses have been studied for a long time. They are defined as follows: we take a configuration at equilibrium at temperature \( T \) (i.e. with a probability distribution proportional to \( \exp(-\beta H) \)) and for each configuration we compute the eigenvalues of the Hessian of the energy, given by eq. (5).

The behaviour of the fraction of INM with negative eigenvalues as the function of the temperature is both interesting and deceiving: interesting because this fraction seems to go to zero near \( T_c \), if we look only to the data above \( T_c \), deceiving because it remains distinctly different from zero also below \( T_c \).

This is exactly what should happens: the spectrum of INM can be computed in mean field theory in simple models [5] and one finds systematically that the spectrum of INM has a part at negative energies both at \( T_c \) and below \( T_c \).

There have been many attempts to get rid of this unwanted part, that exists also in crystals; for example a very interesting observation is that most of the negative eigenvalues at \( T < T_c \) are not related to existence of two different minima, i.e. if we start the minimization of \( H \) moving in one of the unstable directions we arrives always the same minimum [6]. It has also been suggested that the distinction among localized and extended normal modes is relevant. In any case we can assume that the INM provide a good approximation to the spectrum of the Hessian of the free energy, and if a small fraction of eigenvalues is removed, we find the expected behaviour with the fraction \( f \) of negative eigenvalues dropping nearly to zero at \( T_c \).
The qualitative behaviour of the fraction of negative eigenvalues ($f$) in a glass for the saddle normal modes (dotted line), for the instantaneous normal modes (full line). In the case of saddles $f$ seems to vanish very near to the dynamical transition $T_c$.

C. The importance of being a saddle

The study of saddle points and of the spectrum of the small fluctuation nearby, i.d. SNM (saddle normal modes) is a recent achievement. The relevance of saddles has been stressed in [7] and the properties of the spectrum have been analyzed in [8].

A saddle is a generic stationary point of the Hamiltonian and it is a solution of the equations

$$\frac{\partial H}{\partial x_i} = \sum_k V'(x_i - x_k) = 0. \quad (8)$$

In other words the force on all the particles is equal to zero on a saddle. The following specializations are available: when all the eigenvalues are positive the saddle is a minimum and when all the eigenvalues are negative it becomes a maximum.

In glasses the number of saddles is exponentially large when the volume goes to infinity. For each configuration $x_i$ we can associate an inherent saddle, i.e. a saddle that is the nearest one to that particular configuration (the details of this definition depend on the precise definition of distance, however it has the nice feature that the quest for saddles near to a given configuration can be implemented numerically in a meaningful way).

At a given temperature we have a probability distribution of the configuration and this naturally induces a probability distribution on the saddles. As far as the inherent saddles should be not too distant from the the original configuration the SNM spectrum should be not too different from the INM spectrum. However this is one of the cases where a small difference matters.

In mean field theory the analytic computation of the SNM spectrum can be done: we find that if we start from a configuration below $T_c$, the nearby configuration is a minimum and the spectrum has a gap; this gap moves toward zero when we approach $T_c$ and in the region where $T > T_c$ the fraction of negative modes becomes different from zero, i.e. we recover the behaviour described in figure (3).

In a surprising way we find numerically the same effect for a fluid: the qualitative behaviour of the fraction $f$ of negative SNM as function of the temperature is shown in fig. (2) (for comparison we shown also the fraction of negative INM). A similar conclusion arise also if we plot the average fraction of negative SNM ($\bar{f}$) as function of the saddle energy. The quantity $\bar{f}$ vanishes just at the energy that correspond to the dynamical transition $T_c$.

The smart reader would now observe that if our starting configuration is taken in the act of jumping from one minimum to an other minimum, it should be near to a saddle with a negative eigenvalue and
therefore the fraction of SNM is never zero, also at low temperature. However it is quite plausible that these activated processes are quite rare and the fraction of negative negative eigenvalues is not zero below $T_c$ but it maybe a rather small number (e.g. $10^{-6}$), which certainly do not affect the overall picture.

The conclusion is that the spectrum of the SNM has just the properties that we supposed for the eigenvalues of the Hessian of the free energy: negative eigenvalues appear in a significative way only above the critical temperature $T_c$. At temperature smaller than $T_c$ the saddles become minima and the SNM coincide with the inherent structure normal modes of the appropriate energy density.

At temperature higher than $T_c$ the properties of the saddles are definitely different form those of the the inherent structures (i.e. the minima of the Hamiltonian that are the nearest to an equilibrium configurations), however when we decrease the temperature toward $T_c$, the inherent saddles loose the negative part of the spectrum and they start to look like minima and their properties becomes the same of those of the inherent structures. Indeed at temperatures lesser than $T_c$ the saddles are minima and the inherent saddles coincide with the inherent structures.

![Graph](image)

**FIG. 3.** The qualitative behaviour of $\mu$ as function of the temperature in mean field approximation for the saddle normal modes (dotted line), for the instantaneous normal modes (full line) and for the inherent structures normal modes (dashed line).

### IV. THE BOSON PEAK

The conclusions of the previous section provide us a natural interpretation for the Boson peak. In this section hand waving physical arguments will be presented, while in the next section we will present a precise and technical analysis that supports the conclusions of this section.

The reader must have noticed that the computations of the spectrum we alluded in the previous section were not done for fluids but only for simplified mode coupling models. This fact has the sad consequence that phonons are absent from the spectrum. In these models the spectral density has a very simple behaviour: it is a semicircle law starting from a value $\mu(T_c)$. The main results we have described in the previous section are the following (see figure 3):

- For the inherent structures $\mu(T)$ is definitively positive below $T_c$, it goes to zero at $T_c$ and it remains zero in the fluid region above $T_c$.
- For instantaneous normal modes $\mu(T)$ is negative in the fluid phase and remains negative at $T_c$ (it may become positive at definitively lower temperatures) and it reach the $\mu(T)$ of the inherent structures when we arrive at zero temperature.
- For the inherent saddles $\mu(T)$ is negative in the fluid case, it goes to zero at $T_c$ and coincide with that of the inherent structures below $T_c$.  

A further piece of information is important. We have already remarked that if we cool the system very fast below $T_c$ in the ideal mean field model the system is frozen in a metastable state. It can be shown (as a consequence of the principle of marginal stability) that in this case the function $\mu(T)$ of the inherent structures (in this case it coincides with that of the inherent saddles) is equal to zero; on the other hand, if we suppose that the system is able to cross barrier of order $\Delta N$, the quantity $\mu$ becomes a continuous positive function of $\Delta$, vanishing at $\Delta = 0$. It is reasonable to assume that the behaviour of real systems is quite similar to that of the mean field theory with a finite $\Delta$, that increase logarithmically when we decrease the cooling rate.

In other words at low temperature at equilibrium the density of states does not touch zero, however it arrives up to zero in the ultrafast quenched state; in the case of slow cooling the spectrum extend up to zero with a small gap. This physical picture implies that a glassy system has an anomalously high density of vibrational excitations at low energies in the low temperature region. It is natural to assume that this excess of low energy vibrations is connected to the Boson peak.

In order to substantiate this claim we should consider systems that have phonons and prove that there is a Boson peak with all the correct physical properties. In the best case one should be able to compute the properties of the Boson peak in a quantitative way. A microscopical approach which tries to obtain these results is described in the next section.

V. A MICROSCOPIC APPROACH

We come back to the original problem stated in the introduction. We would like to compute the spectrum of the matrix $M$ associated to the quadratic form

$$\frac{1}{2} \sum_{i,k} h(x_i - x_k)(\phi_i - \phi_k)^2.$$  \hspace{1cm} (9)

This matrix has interesting properties; translational invariance predicts the presence of a phononic spectrum with density of states $\rho(z)$ that at small eigenvalue $z$ is greater or equal to $z^2$ in three dimensions.

The most interesting situation happens in the case of a non positive $h$. Here negative eigenvalues are possible. A very simple probabilistic argument shows that in the infinite volume limit a generic configuration of the $x$'s always has negative (may be localized) eigenvalues.

We can argue that there are two phases:

- The **phonon** phase, where negative eigenvalues are localized. Here the spectral density goes approximately like $z^{1/2}$ at small (but not small) $z$.

- The **saddle** phase where negative eigenvalues are present and the spectral density goes like a constant at small $z$.

However in a first approximation the density of localized eigenvalues is small. If we neglect them, we can state that in the phonon phase negative eigenvalues are absent and the spectral density goes like $z^2$ at small $z$.

Let us consider the case where the function $h(x)$ depends on a parameter $g$ that we can tune in such a way that for $g > g_c$ we are in the phonon phase, while for $g < g_c$ we are in the saddle phase. We would like to show that a Boson peak is present in the phonon case in the region of $g$ near to $g_c$. In other words, if we consider a matrix of the form given in eq. (9), we expect that when this matrix is loosing its stability (i.e. we are near to $g_c$) a Boson peak appear. The Boson peak is therefore an universal feature of random matrices near the phonon-saddle transition and its properties should not depends too much on the microscopic details.

In order to prove this statement we have to make a microscopic computation of the spectrum and of the eigenvectors and to show that near $g_c$ a Boson peak is present. The simplest way to reach this goal is to extend the CPA (coherent potential approximation) approach, (that works very well on the lattice) to off-lattice models.

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2These states are also connected with dynamic heterogeneities in cooling, but this relation cannot be discussed here for reasons of space.
Usually in the CPA approach the density of states is well approximated, however localized states are absent and one finds a zero density of states at places where the density of states is very small. This drawback of the CPA is useful in our case because it gives an exactly zero density of states in the phonon phase at negative eigenvalues \((z)\).

The generalization of the CPA to our case is not so simple and it has been obtained after a long series of works \([9,10]\). Let me be rather sketchy on this point. The crucial step consists in introducing (as usual) the resolvent

\[
R(j, k|z) \equiv \left(\frac{1}{z - M}\right)_{j,k}.
\]

The Green function is the average of the resolvent, i.e.

\[
G(p, z) = \sum_{j,k} R(j, k|z) \exp(i(x_j - x_k)).
\]

The Green function is related to the usual structure function by the relation:

\[
S(p, z) \propto p^2 z^{-1} \text{Im} \, G(p^2, z^2 + i0^+) \quad (12)
\]

With some effort \([10]\) one can derive an approximate integral equation for the resolvent which looks like

\[
G(p, z)^{-1} = G_0(p, z)^{-1} - \Sigma(p, z),
\]

\[
\Sigma(p, z) = \int d^3q W(p, q) G(q, z) \quad (13)
\]

with an appropriate definition of the bare Green function \(G_0(p, z)\) and of the vertex \(W(p, q)\). These equations are similar to those derived using a completely different approach in the framework of the mode coupling theory \([11]\), however the form of the vertex is rather different and this leads to subtle differences that cannot be discussed here.

A detailed computation \([10]\) shows that the previous integral equations do have a transition from a phonon phase to a saddle phase and that a Boson peak is present near the transition in the phonon phase. The discussion of the the comparison with scattering experiments and their relevance in the framework of the glass transition cannot be done here for reasons of space and can be found in \([10]\).

We can this conclude that a Boson peak is a generic property of translational invariant matrices which are near the phonon-saddle transition and this phenomenon is not restricted to glasses. On the contrary it is the duty of the theory of glasses to explain why glasses at low temperature are near to the phonon-saddle transition and modern theories of glasses have a clear explanation for this phenomenon.

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