Boson peak in two-dimensional random matrix models

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Abstract. We present a stable random matrix approach to the old standing problem of the boson peak in amorphous dielectrics (glasses). In this paper, we consider a two-dimensional case. We show that in the 2d case the boson peak in the density of vibrational states appears in a natural way in different random matrix models similar to the 3d case. Changing the parameters of random matrices one can shift the boson peak to higher or to lower frequencies depending on the strength of disorder in the model. In all investigated cases the position of the boson peak is correlated with the Young modulus of the lattice.

1. Introduction

It is well known that all glasses independently of their chemical composition have universal properties in a wide range of frequencies (or temperatures) [1]. One of these properties is a well-known boson peak in the reduced density of vibrational states $g(\omega)/\omega^{d-1}$, where $d$ is a space dimension [2]. It characterizes an additional to Debye vibrational density at low frequencies far below the Debye frequency.

This peak is well seen in the measurements of the heat capacity, in the light and X-ray scattering, and in the inelastic neutron scattering. The boson peak frequency $\omega_b$ is correlated with Ioffe-Regel crossover frequency $\omega_{IR}$ when the phonon mean free path becomes of the order of the phonon wavelength [3, 4, 5, 6, 7]. Despite a big number of articles about the boson peak, its physical origin is still unclear. In the present paper, we apply a new approach to the boson peak problem based on random matrices. We show that in many random matrix models the boson peak appears in a natural way.

2. Random matrix model

The symmetric dynamical matrix $M$ determines the eigenfrequencies squared. It is natural to suppose that in amorphous solids due to local disorder the dynamical matrix has some disorder as well. It also has some general regular properties. First of all, it has translational symmetry [8]. In a scalar model with equal atomic masses $m_i = 1$, the sum of elements in each row and each column of the matrix $M$ should be zero

$$\sum_{i=1}^{N} M_{ij} = \sum_{j=1}^{N} M_{ij} = 0,$$  \hspace{1cm} (1)
where \( N \) is the number of atoms. Secondly, the translation invariance conditions (1) are necessary but not sufficient for existing low-frequency acoustic modes (acoustic phonons) in amorphous solids. For existing of these modes, one needs nonzero macroscopic rigidity (Young modulus). Finally, the matrix \( M \) should be mechanically stable. It means that all eigenfrequencies squared should not be negative. Then in such a system in the framework of standard elasticity theory the low-frequency sound wave can propagate. We consider below three different simplest two-dimensional scalar models (but sufficiently general) where all these conditions are satisfied and we have a boson peak in the reduced density of states \( g(\omega)/\omega \).

The mechanical stability of the random symmetric matrix \( M \) is guaranteed if we take it in the form [9]

\[
M = AA^T. \tag{2}
\]

Here \( A \) is some real and not necessary symmetric matrix. In the simplest case, the matrix \( A \) is a square \( N \times N \) random matrix. For simplicity let us build this matrix \( A \) on a quadratic lattice (with lattice constant \( a_0 = 1 \)) with identical atoms in the nods. Let us take into account the interaction between nearest neighbors only [9]. Non-zero non-diagonal matrix elements \( A_{ij} \) for nearest neighbors \( i \) and \( j \) are random Gaussian values with unit variance and zero mean. The diagonal elements are defined as

\[
A_{kk} = -\sum_{i \neq k} A_{ik} \tag{3}
\]

to satisfy the condition of the translational invariance (1).

As a result, we have satisfied the most important properties of the dynamical matrix \( M \). Nevertheless, the acoustic phonons can not propagate in this lattice and there is no boson peak in the density of states. The reason is that the Young modulus of the lattice is zero and the system has zero rigidity in the thermodynamic limit. The same takes place in the 3d case [10].

3. Bond counting

According to the Maxwell counting rule [11], the above-mentioned system is isostatic [12]. As a result, it is critically soft and has zero macroscopic rigidity. It follows from the point that the number of degrees of freedom \( N \) is exactly equal to the number of bonds \( K \). Indeed, using the dynamical matrix \( M \) we can write the potential energy of the system \( U \) as a quadratic form of atomic displacements from the equilibrium, \( u_i \) \((i = 1...N)\)

\[
U = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} M_{ij} u_i u_j. \tag{4}
\]

Since the dynamical matrix \( M \) can be presented as a product (2), the potential energy \( U \) can be written as a sum over \( k \) of \( N \) quadratic terms

\[
U = \frac{1}{2} \sum_{k=1}^{N} \left( \sum_{i=1}^{N} A_{ik} u_i \right)^2. \tag{5}
\]

It proves that the quadratic form (4) is positive definite. Summation over \( rows \) of the matrix \( A \) in Eq. (5) is taken over \( i \) from 1 to \( N \), which is the number of atoms or the number of degrees of freedom (in the scalar model). Summation over \( columns \) of the matrix \( A \) in Eq. (5) is taken over \( k \) from 1 to \( N \). Therefore, the index \( k \) enumerates different quadratic terms.

Each quadratic term in the potential energy \( U \) is determined by some column of the matrix \( A \) and can be considered as a mechanical bond (in a general sense) in the system [13]. The number of these bonds \( K \) is the number of columns in the matrix \( A \). In our scalar model, it
coincides with the number of atoms $N$, i.e. with the number of degrees of freedom since the matrix $A$ is a square matrix. Therefore, the system $M = AA^T$ with the random square matrix $A$ is mechanically stable but has zero macroscopic rigidity.

To make our system macroscopically rigid one must add additional bonds. Since each bond corresponds to some column in the matrix $A$ we must increase the number of columns in the matrix $A$ and make $K > N$. As a result, the square $N \times N$ matrix $A$ becomes a rectangular $N \times K$ matrix $A$. In order to increase the number of bonds, one can add to the matrix $AA^T$ some other square matrix $N \times N$ which is translational invariant. The sum of these two matrices will have finite rigidity. It can be done in many ways. We consider below three of them.

4. Three random matrix models with non-zero rigidity

First method. Let us take the dynamical matrix $M$ in the form

$$ M = \mathcal{A} \mathcal{A}^T = AA^T + \mu M_0. \quad (6) $$

Here $A$ is the same square random matrix $N \times N$, built on a quadratic lattice and having translation invariance. The matrix $M_0$ is a regular crystalline dynamical matrix $N \times N$, built on the same lattice with unit springs between nearest neighbors and having non-zero rigidity. The parameter $\mu \geq 0$ is a rigidity of these springs. If $\mu = 0$ we go back to the previous case (2) of the system with zero rigidity.

It is easy to check without writing of the exact form of the rectangular matrix $\mathcal{A}$, that its number of rows is equal to $N$ (i.e. to the number of degrees of freedom). The number of columns (i.e. the number of bonds) is equal to $3N$: $N$ columns are columns of the matrix $A$, and additional $2N$ columns (bonds) are determined by the crystalline matrix $M_0$. As a result, the matrix $\mathcal{A}$ is $N \times 3N$ matrix. We have shown that the Young modulus $E$ in this system for $\mu > 0$ is different from zero and $E \propto \sqrt{\mu}$ (for $\mu \ll 1$). Therefore, phonons can propagate in this lattice.

Normalized to unity the density of states $g(\omega)$ for the model (6) is shown in Fig. 1(a) for $N = 1000^2$ and different values of the parameter $\mu$. We used the Kernel Polynomial Method (KPM) to calculate the density of states [14]. The straight lines show the Debye contribution

$$ g_D(\omega) = \frac{1}{2\pi E} \omega, \quad (7) $$
calculated using the Young modulus $E(\mu)$ for non-zero values of $\mu$.

In the case of $\mu = 0$ we obtain the density of states of non-rigid $M = AA^T$ system, $g_0(\omega)$. It does not satisfy the Debye law (7) with any value of the Young modulus. One can show that $g_0(\omega)$ has a logarithmic singularity at $\omega = 0$.

The reduced density of states $g(\omega)/g_D(\omega)$ shows the boson peak for nonzero values of the parameter $\mu$ (Fig. 1(d)).

Second method. Let us write the matrix $M$ as

$$ M = \mathcal{A} \mathcal{A}^T = AA^T + M_0(p). \quad (8) $$

It is different from the previous case. Now $\mu = 1$ and all springs in the crystalline matrix $M_0$ have unit rigidity. To decrease the number of bonds we randomly cut out springs from the matrix $M_0$. The cutting out of one spring is equivalent to removing of one bond, i.e. one column of the matrix $\mathcal{A}$. The part of remaining springs in the system is denoted by $p$. The matrix $M_0$ with cut out springs is denoted by $M_0(p)$. It is easy to see that the matrix $\mathcal{A}$ has $N$ rows and $N(1 + 2p)$ columns. We have shown that the Young modulus $E(p)$ in this system for $p > 0$ is different from zero and phonons can propagate in the system. We have shown that the Young modulus $E \propto p$ for $p \ll 1$. 

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Figure 1. Left column: (a), (b), and (c) show the normalized to unity density of states \(g(\omega)\) for three random matrix models (6), (8) and (9) respectively and different values of parameters \(\mu\), \(p\) and \(\beta\). The random matrix \(A\) was built on the quadratic lattice with periodic boundary conditions and \(N = 1000^2\). The straight lines show the Debye density of states (7) with independently calculated values of Young modulus for each of three random matrix models and different values of the above-mentioned parameters. Right column: (d), (e), and (f) show the boson peaks in the reduced density of states \(g(\omega)/g_D(\omega)\) calculated from the density of states \(g(\omega)\), shown in (a), (b), and (c) respectively.

Normalized to unity the density of states \(g(\omega)\) in this model is shown in Fig. 1(b) for different values of the parameter \(p\). The straight lines show the Debye contribution (7) calculated from the Young modulus \(E(p)\). The case \(p = 0\) corresponds to the density of states of the non-rigid system, \(g_0(\omega)\). The boson peak in the reduced density of states \(g(\omega)/g_D(\omega)\) is shown in Fig. 1(e) for non-zero values of \(p\).

Third method. Let us take the matrix \(M\) in the form

\[
M = AA^T = AA^T + \beta BB^T.
\]

(9)

Here \(A\) is again the same random \(N \times N\) matrix built on a quadratic lattice and having
translational invariance. The matrix $B$ is independent from $A$ random $N \times N$ matrix made by the same rules as the matrix $A$. The parameter $\beta \geq 0$ can vary. For $\beta = 0$ we come back to the case of non-rigid system (2).

It is easy to see that the number of rows in the matrix $A$ is equal to the number of degrees of freedom $N$ as before, and the number of columns (i.e. the number of bonds) is equal to $2N$. It is clear that $N$ bonds (columns) come from the matrix $A$, and $N$ bonds come from the matrix $B$. We have shown that there are phonons in such a system since Young modulus for $\beta > 0$ is different from zero and $E \propto \sqrt{\beta}$ (for $\beta \ll 1$). It is interesting to note that each term in Eq. (9) taken separately has zero rigidity but together the Young modulus is different from zero.

Normalized to unity the density of states $g(\omega)$ in this model is shown in Fig.1(c) for different values of the parameter $\beta$. The straight lines show the Debye contribution (7) which was calculated from the Young modulus $E(\beta)$ for non-zero values of $\beta$. The case $\beta = 0$ corresponds to the density of states of the non-rigid system, $g_0(\omega)$. The boson peak in the reduced density of states $g(\omega)/g_{D}(\omega)$ is shown in Fig.1(f) for non-zero values of $\beta$.

5. Boson peak frequency

![Figure 2. The correlation of the boson peak frequency $\omega_b$ and Young modulus $E$ in three considered random matrix models for four different values of parameters $\mu$, $p$ and $\beta$ shown in Fig.1.](image)

As follows from the analysis of the data, the boson peak frequency $\omega_b$ is correlated with the Young modulus of the lattice $E$. Figure 2 shows positions of the boson peak $\omega_b$ in three considered matrix models (6), (8) and (9) together with the corresponding Young modulus value $E$ for four non-zero values of parameters $\mu$, $p$ and $\beta$. As follows from this figure, the boson peak frequency $\omega_b$ is proportional to the corresponding Young modulus value $E$ in all considered cases.

$$E \sim \omega_b.$$ (10)

The same behavior was obtained in the 3d case of the same random matrix models [13]. A similar correlation between the boson peak $\omega_b$ and the shear modulus $G$ was observed in the granular medium near the jamming transition point [15]. At this point the shear modulus goes to zero. The correlation between boson peak frequency and the shear modulus was also observed experimentally in modified borate glasses [16]. This correlation makes it possible to explain qualitatively in a unique way the physical origin of the boson peak in our random matrix models.
On the one hand, at low frequencies $\omega < \omega_b \ll 1$ the density of states $g(\omega)$ is given by the Debye contribution $g_D(\omega b)$. Taking into account that $\omega b \sim E$, we get $g_D(\omega b) \sim 1$. On the other hand, at high frequencies $\omega > \omega_b$ the density of states $g(\omega)$ is approximately $g_0(\omega)$ as follows from Fig.1. However, these two asymptotics have different values at $\omega = \omega_b$ since $g_0(\omega_b)$ logarithmically diverge at $\omega = 0$. For small enough values of $\omega_b$, the value of $g_0(\omega_b)$ should overcome the constant value of $g_D(\omega b)$. Such behavior is responsible for the peak in the reduced density of states, which height is determined by the ratio $g(\omega_b)/g_D(\omega_b) \sim g_0(\omega_b)$. The height of the peak logarithmically grows with decreasing of $\omega_b$. Such behavior differs from the 3d case [13], where the height of the peak has the power-law behavior.

Summarizing, we have shown that the boson peak appears naturally in different models of stable random matrices with translational invariance under rather general conditions applied to the system. In all investigated cases the boson peak frequency is proportional to the Young modulus of the system. According to the 3d model investigated in more details in [10], the boson peak in the 3d model appears at frequencies around Ioffe-Regel crossover frequency. The phonons experience strong scattering on quasilocal vibrations and, as a result, transforms to diffusons. In other words, near the boson peak the character of propagation of vibrational modes is changing drastically [10]. In the 2d model, the density of states is similar to the 3d model: the boson peak frequency is the crossover between the Debye law $g_D(\omega)$ and the high-frequency density of states $g_0(\omega)$. Therefore, there is reason to believe that the character of vibrations in all our 2d model is similar to the 3d model. The detailed calculations of the vibrational properties will be presented in a subsequent paper.

One of the authors (Y.M.B.) thanks the Dynasty Foundation and the Council for grants of the President of the Russian Federation (grant SP-3299.2016.1) for the financial support.

References
1. D. A. Parshin, Phys. Solid State 36, 991 (1994).
2. V.L. Gurevich, D.A. Parshin, H.R. Schober, Phys.Rev. B, 67, 094203, (2003).
3. V.L. Gurevich, D.A. Parshin, J. Pelous and H.R. Schober, Phys.Rev. B 48, 16318 (1993).
4. D.A. Parshin and C. Laermans, Phys.Rev. B, 63, 132203 (2001).
5. B. Rufflé, G. Guimbretière, E. Courtens, R. Vacher and G. Monaco, Phys.Rev.Lett. 96, 045502 (2006).
6. B. Rufflé, D.A. Parshin, E. Courtens and R. Vacher, Phys.Rev.Lett. 100, 015501 (2008).
7. H. Shintani and H. Tanaka, Nature Materials 7, 870 (2008).
8. A.A. Maradudin, E.W. Montroll, G.H. Weiss, and I.P. Ipatova, Theory of Lattice Dynamics in the Harmonic Approximation (Academic Press, New York, 1971).
9. Y. M. Beltukov and D. A. Parshin, JETP Lett. 93, 598 (2011)
10. Y.M. Beltukov, V.I. Kozub, D.A. Parshin, Phys.Rev.B, 87, 134203 (2013).
11. J.C. Maxwell, Philosophical Magazine 27, 294 (1865).
12. C.S. O’Hern, L.E. Silbert, A.J. Liu, S.R. Nagel, Phys. Rev. E 68, 011306 (2003).
13. Y. M. Beltukov, D. A. Parshin, JETP Letters 104, 552 (2016).
14. Y.M. Beltukov, C. Fusco, D. A. Parshin, A. Tanguy, Phys.Rev.E, 93, 023006, (2016).
15. V. Vitelli, N. Xu, M. Wyart, A. J. Liu, S. R. Nagel, Phys.Rev.E 81, 021301 (2010).
16. S. Kojima, M. Kodama, Physica B: Cond. Mat. 263, 336 (1999).