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Quasi-local vibrations in amorphous solids in the framework of the theory of non-Gaussian random matrices

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The statistical features of quasi-local vibrations of disordered systems are studied within the framework of the model of correlated random matrices. It is shown that the statistics of matrix elements of the dynamical matrix strongly affects the properties of such vibrations. The lowest frequency part of the density of states of quasilocal vibrations is described by the expression $\rho_{\text{qlv}}(\omega) \propto \omega^n$, where the power n is the number of neighboring atoms. However, if the distribution of matrix elements is strongly non-Gaussian, an additional dependence $\rho_{\text{qlv}}(\omega) \propto \omega^\gamma$ appears, where the power γ decreases as the degree of non-Gaussianity increases.

Keywords: quasi-local vibrations, amorphous solids, random matrices.

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1. Introduction

Low-frequency properties of amorphous materials and nanocomposites on their basis differ significantly from the properties of corresponding crystal counterparts, thanks to which such materials, disordered throughout the volume, are of the greatest interest. It is currently known that the low-frequency part of vibrational states of amorphous dielectrics is caused by different vibration types [1,2]. Phonons, as vibrations with a relatively large mean free path, are accountable for the lowest-frequency properties of disordered mechanical systems. As the frequency increases, the phonon wavelength becomes comparable to their mean free path, which leads to the replacement of phonons by another type of vibrational excitations–diffusons, which propagate through the system by diffusion energy transfer The phonon to diffuson transition is known as the Ioffe–Regel crossover [3].

The Ioffe–Regel crossover in amorphous materials occupies some frequency range. First of all, this is due to the fact that phonons experience an additional scattering on different vibration types. One of such types are vibrations of anomalously soft regions of amorphous media called quasi-local vibrations. These are vibrations of a group of atoms weakly bounded to their environment [2]. Soft regions are formed in amorphous materials during their glass transition Therefore, quantity and properties of quasi-local vibrations are considerably affected by glass cooling processes.

Quasi-local vibrations are a subject of intensive research. It was shown in [4–6] that quasi-local vibrations determine the main contribution to the scattering of acoustical phonons at frequencies of about 1 THz. Studies of highly supercooled model glasses show that the properties of quasi-local vibrations do not depend on the parameters of spatial scale [7,8], rate and protocols of structure cooling [9–11]. Thereat, density of quasi-local states is $\rho_{\text{qlv}}(\omega) \propto \omega^\gamma$, $\gamma \approx 4$ for most of the studied systems [7,12,13].

That's why it is difficult to distinguish the contribution of quasi-local vibrations to density of states in conventional amorphous systems from Rayleigh scattering of phonons on disorder [7–14], which complicates their studies.

To date, the question of the relationship between quasi-local vibrations and correlated disorder, which is an important attribute of amorphous media, has not been studied yet. As a result of cooling, certain regions of an amorphous structure reach the metastable equilibrium position which is near the stability loss. Due to microscopical disorder of glass, this leads to a strong correlation of force constants and internal frustration [15,16]. In this regard, the presence of correlations between force constants should be taken into account when studying quasi-local vibrations.

Small atomic vibrations near the stable equilibrium position are described by the dynamic the matrix M, which is nonnegative definite and can always be represented as

$$\hat{M} = \hat{A}\hat{A}^T. \tag{1}$$

This representation allows for automatic consideration of the mechanical stability requirement, since all eigenvalues of $\hat{M}$, which correspond to squared eigenfrequencies, are nonnegative, and for using the Wishart ensemble to describe the vibrational properties in terms of the random matrix theory [17,18]. The matrix elements A_{ij} in such an ensemble are random numbers with a certain distribution, with are correlated with each other due to the sum rule, which has the following form for the case of identical atomic masses in the scalar model [19]:

$$\sum_i A_{ij} = 0. \tag{2}$$

This rule corresponds to the condition of translation symmetry of a mechanical system $\sum_i M_{ij} = 0$, which ensures the presence of low-frequency vibrations as plane waves which obey the Debye law [17]. This approach made it possible to describe the phonon to diffuson transition and the nearby boson peak [17–19]. However, there is the open question of quasi-local vibrations in this model and their relation to statistical peculiarities of elements of the matrix $\hat{A}$. The present paper answers these questions.

2. Soft modes in the random matrix model

Matrix $\hat{A}$ in the considered model of random matrices (1) describes the coupling between different degrees of freedom in the system. Each row of the matrix $\hat{A}$ corresponds to a degree of freedom, while each column corresponds to a bond between several degrees of freedom with quadratic potential energy [19]. For simplicity, in the present paper we consider a scalar model of atomic displacements, therefore the number of degrees of freedom is equal to number of atoms N. If the number of bonds is $K \geq N$, then the system has macroscopic stiffness. The main parameter in the considered model is $\varkappa = (K - N)/N$, which can vary in wide range $0 \leq \varkappa < \infty$. The case $\varkappa \ll 1$, which corresponds to a system with a large fluctuation of force constants, is of the greatest interest.

Matrix $\hat{A}$ can be constructed on a regular lattice, if atoms are arranged at its sites according to the following rules. In the case of a quadratic the matrix $\hat{A}$, its the matrix element A_{ij} is a non-zero random number, only if atoms with indices i and j are the nearest neighbors. Such a consideration corresponds to a local fluctuation of force constants, which is observed in amorphous materials which have only the short-range order in the atomic arrangement. For simplicity, it will be considered that each atom has an identical number of neighbors n. Diagonal element $A_{ii} = -\sum_{j \neq i} A_{ji}$ ensures the sum rule (2). Thus, each row in a quadratic the matrix $\hat{A}$ has $n + 1$ non-zero numbers: n random independent numbers and 1 number equal to the sum of other n independent random numbers.

In case of $0 < \varkappa \leq 1$, a rectangular the matrix $\hat{A}$ can be obtained from two different realisations of a quadratic the matrix: $\hat{A}^{(0)}$ and $\hat{A}^{(1)}$. In this case, the resultant rectangular the matrix $\hat{A}$ is constructed by adding $\varkappa N$ randomly chosen columns of the matrix $\hat{A}^{(0)}$ to the matrix $\hat{A}^{(1)}$ on the right.

When constructing the matrix $\hat{A}$, there is a probability that all the numbers present in some of its rows have small values. This corresponds to the fact that these atoms are weakly bounded to their environment. Frequencies of such quasi-local vibrations ω_{qlv} will lie in the low-frequency region of the spectrum and be described by a certain distribution density $\rho_{\text{qlv}}(\omega)$, which is related to the statistics of the matrix elements A_{ij}.

Let us find the density of states of quasi-local vibrations $\rho_{\text{qlv}}(\omega)$ using the perturbation theory methods. Let us assume that the row of the matrix $\hat{A}$ with index l contains small numbers. It will be also assumed that the matrix elements A_{lj} at $j > N$ are zero. The probability of such a case is equal to $(1 - \varkappa)^{n+1}$. Then the matrix $\hat{A}$ can be represented as follows:

$$\hat{A} = \hat{A}_0 + \hat{V}. \tag{3}$$

All row elements with index l in the matrix $\hat{A}_0$ are zero. On the contrary, the matrix $\hat{V}$ contains non-zero elements only in the row with index l: n non-zero independent numbers $v_1, \ldots, v_n$ and one correlated number $v_{n+1} = V_{ll} = -\sum_{i \neq l} (\hat{A}_0)_{il}$.

The frequency of quasi-local vibration ω_{qlv} in the second order of the perturbation theory is determined by the following expression:

$$\omega^2_{\text{qlv}} = \left\{ \hat{V} \hat{H} \hat{V}^T \right\}_{ii}, \tag{4}$$

where

$$\hat{H} = \hat{I} - \hat{A_0}^T \left(\hat{A}_0 \hat{A_0}^T \right)^{-1} \hat{A}_0, \tag{5}$$

and $\hat{I}$ is a unity matrix of the size $K \times K$ [20]. It follows from expression (4) that ω^2_{qlv} is a sum of quadratic forms of $n + 1$ numbers $v_1, \ldots, v_{n+1}$, which correspond to non-zero elements V_{lj}. Therefore, a symmetrical matrix can be introduced for further convenience

$$\hat{C} = \hat{P} \hat{H} \hat{P}^T, \tag{6}$$

where $(n + 1) \times K$ matrix $\hat{P} \times$ has non-zero the matrix elements $P_{kj} = 1$ only for the indices at which $V_{lj} = v_k$. Then the quasi-local vibration frequency is determined by the following expression:

$$\omega_{\text{qlv}} = \sqrt{v \hat{C} v^T}, \tag{7}$$

where row vector $v = v_1, \ldots, v_{n+1}$ is composed of non-zero elements V_{lj}.

Since each index l corresponds to its own set of the values of v, quasi-local vibrations have a spread in frequency (7). Thereat, the low-frequency part of spectrum $\omega \ll 1$ in small-size systems is due to quasi-local vibrations. The number of phonons in such systems is small because their minimum vibration frequency is limited by the system sizes. This makes it possible to distinguish the phononic density of states from the distribution density of quasi-local vibrations.

3. Influence of statistics of matrix elements

Frequency distribution (7) for a set of $n + 1$ random values of v at $\omega_{\text{qlv}} \ll 1$ is found in Appendix 1. Distribution density of quasi-local vibrations $\rho_{\text{qlv}}(\omega)$ has the following form:

$$\rho_{\text{qlv}}(\omega) = (1 - \varkappa)^{n+1} p \omega^n, \tag{8}$$

where the coefficient is

$$p = \left\langle \det(\hat{C})^{-1/2} \right\rangle \frac{2\pi^{\frac{n+1}{2}}}{\Gamma\left(\frac{n+1}{2}\right)} \prod_{k=1}^{n+1} \rho_k(0). \qquad (9)$$

The angle brackets correspond to averaging over different realisations of the matrix $\hat{A}_0$, Γ is the gamma function, $\rho_k(0)$ corresponds to the distribution density of random value v_k near zero.

The coefficient p does not depend on the system parameter $\varkappa$. With small $\varkappa \ll 1$, the elements of the matrix $\hat{C}$ are proportional to $\varkappa$, therefore

$$\left\langle \det(\hat{C})^{-1/2} \right\rangle \propto \varkappa^{-\frac{n+1}{2}}. \qquad (10)$$

Thus, at $\varkappa \ll 1$ the coefficient $p \propto \varkappa^{-\frac{n+1}{2}}$.

The coefficient p also depends on the statistics of the matrix elements A_{ij}. For simplicity, we will assume that the matrix elements A_{ij}, corresponding to an interaction with the nearest neighbors, are distributed independently with an equal dispersion σ^2 and zero mean.

3.1. Gaussian statistics

In the case of Gaussian statistics of the matrix elements A_{ij}, numbers v_k obey a multidimensional Gaussian distribution

$$\rho(v) = \frac{1}{\sqrt{(2\pi)^{n+1} \det \hat{\Xi}}} e^{-\frac{1}{2} v \hat{\Xi}^{-1} v^T}, \qquad (11)$$

where $\Xi_{km} = \langle v_k v_m \rangle$ is a covariance matrix which in the considered case of an independent distribution of random numbers has a diagonal form: $\Xi_{km} = \sigma_k^2 \delta_{km}$. Then the probability density function of random value v_k near zero has the following form:

$$\rho_k(0) = \frac{1}{\sqrt{2\pi}\sigma_k}. \qquad (12)$$

The standard deviation for $k \le n$ is $\sigma_k = \sigma$. However, the standard deviation for $k = n+1$ is $\sigma_{n+1} = \sqrt{n}\sigma$, since value v_{n+1} is a sum of n independent Gaussian numbers. Taking this into account, coefficient (9) has the following form:

$$p = \left\langle \det(\hat{C})^{-1/2} \right\rangle \frac{2^{\frac{1-n}{2}}}{\Gamma\left(\frac{n+1}{2}\right) \sigma^{n+1} \sqrt{n}}. \qquad (13)$$

3.2. Non-Gaussian statistics

Values of amplitudes of force constants in different regions of real amorphous materials can differ by several orders [15]. To achieve such a spread, we will assume that the independent non-zero elements of the matrix $\hat{A}$ have a non-Gaussian distribution which is assigned as

$$v_k = c\eta_k \exp \xi_k, \quad k \le n, \qquad (14)$$

where η_k is a random number which has a Gaussian distribution with a zero mean and a unit dispersion, ξ_k is a random number uniformly distributed from $-b/2$ to $b/2$. Normalization constant $c = \sigma\sqrt{b/\sinh(b)}$ determines dispersion $\langle v_k^2 \rangle = \sigma^2$.

The probability density function of quantity (14) has the following form:

$$\rho(v_k) = \frac{\operatorname{erf}\left(\frac{e^{b/2}}{\sqrt{2}c} v_k\right) - \operatorname{erf}\left(\frac{e^{-b/2}}{\sqrt{2}c} v_k\right)}{2bv_k}. \qquad (15)$$

Parameter b determines the degree of non-Gaussianity of the distribution of v_k. The distribution of random value v_k at $b \ll 1$ is close to a Gaussian one with a zero mean and dispersion σ^2.

Element v_{n+1} is determined by the sum rule (2), therefore it is a sum of n independent random numbers constructed according to rule (14). Therefore, it follows from formula (15) that

$$\rho_k(0) = \sqrt{\frac{2}{\pi}} \frac{1}{bc} \sinh\frac{b}{2}, \quad k \le n,$$

$$\rho_{n+1}(0) = \frac{1}{\sqrt{2\pi}\, c} \left\langle \left(\sum_{i=1}^{n} e^{2\xi_i} \right)^{-1/2} \right\rangle_{\xi}, \qquad (16)$$

where the angle brackets correspond to the averaging over different random numbers ξ_i uniformly distributed from $-b/2$ to $b/2$. The value of $\rho_{n+1}(0)$ can be calculated numerically for any value of the parameter b and number of neighbors n. Taking into account expression (16), coefficient (9) becomes as follows:

$$p = \left\langle \det(\hat{C})^{-1/2} \right\rangle \frac{2^{\frac{1-n}{2}}}{\Gamma\left(\frac{n+1}{2}\right) c^{n+1}} \times \left(\frac{2}{b} \sinh\frac{b}{2} \right)^n \left\langle \left(\sum_{i=1}^{n} e^{2\xi_i} \right)^{-1/2} \right\rangle_{\xi}. \qquad (17)$$

In Figures 1 and 2 the obtained analytical result for the density of states of quasi-local vibrations (8) is compared with the numerical calculation of density of states $\rho(\omega)$ for the entire system. Density of states $\rho(\omega)$ was found by the full diagonalization of dynamic matrix $\hat{M} = \hat{A}\hat{A}^T$ for the case of Gaussian statistics of the elements of the matrix $\hat{A}$ (Fig. 1) and for the case of their non-Gaussian statistics (Fig. 2). To do so, the matrix $\hat{A}$ was constructed on a simple cubic lattice sized $14 \times 14 \times 14$ with the lattice constant $a_0 = 1$ and atomic masses $m_i = 1$, and a unity dispersion of the matrix elements $\sigma^2 = 1$ is considered. The number of neighboring atoms in case of a simple cubic lattice is $n = 6$. A numeric diagonalization of 10^8 random matrices was performed to plot the histograms.

The solid lines in Figures 1 and 2 show a good agreement of the low-frequency density of quasi-local states (8) with the numerical calculation result, both in the case of Gaussian (Fig. 1) and non-Gaussian statistics (Fig. 2). Here the

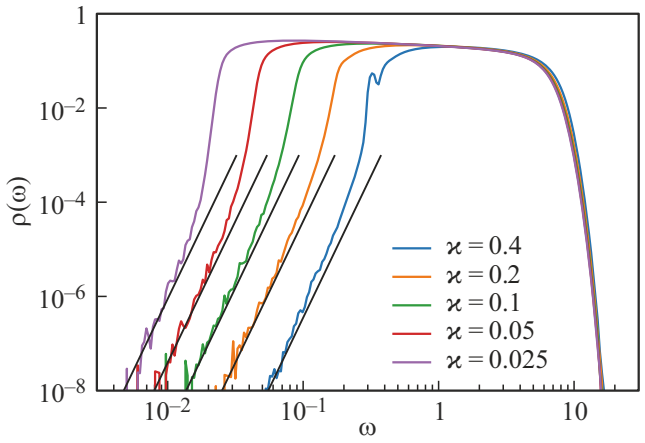

Figure 1. The vibrational density of states in the case of a Gaussian distribution of elements of the matrix $\hat{A}$ with dispersion $\sigma^2 = 1$ for different parameters $\varkappa$. The lines show the low-frequency contribution of quasi-local vibrations (8).

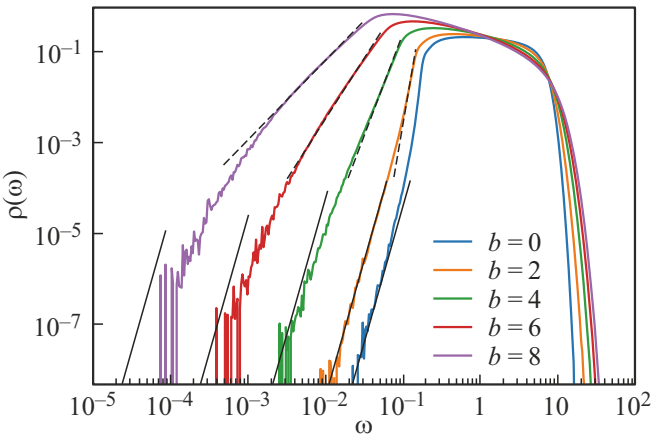

Figure 2. The vibrational density of states in the case of a non-Gaussian distribution of elements of the matrix $\hat{A}$ with dispersion $\sigma^2 = 1$ for different the parameters b. The parameter $\varkappa = 0.2$. The solid lines show the low-frequency dependence (8), the dashed lines show the result for a strongly non-Gaussian distribution (23).

frequency range in which the power-law dependence ω^n is satisfied depends both on the parameter κ and on the non-Gaussian the parameter b. The region where dependence ω^n is met for strongly non-Gaussian statistics ($b > 4$) is outside the capabilities of numerical counting. It should be noted that the coefficient preceding the power dependence ω^n was calculated using formula (8) and was not a fitting parameter. Thus, the solid lines in Fig. 2 are low-frequency asymptotics for any value of the parameter b.

Thus, we can draw the conclusion that the lowest-frequency part of density of states in this model of random matrices is due to quasi-local vibrations and has power dependence $\rho_{\text{qlv}}(\omega) \propto \omega^n$, where the power n is the number of neighboring atoms.

4. Strongly non-Gaussian statistics

In case of $b \gg 1$, the statistics of matrix elements is strongly non-Gaussian and the distribution density of quasi-local states has a non-trivial power dependence in the intermediate frequency range (see the dashed lines in Fig. 2). Values of v_k in this case has an exponentially large spread, therefore frequency (7) is determined by the largest value of v_k:

$$\omega_{\text{qlv}} \approx \max_k |v_k|. \tag{18}$$

Such an approximation acts well in the frequency range $\omega_0 \ll \omega \ll \omega_1$, where $\omega_0 = ce^{-b/2}$ and $\omega_1 = ce^{b/2}$. The previously obtained result (8) is applicable at lower frequencies $\omega \ll \omega_0$.

In order to find the frequency distribution (18) in case of $b \gg 1$, we can omit the random Gaussian quantities η_k in expression (14) and assume that $|v_k| \approx c \exp \xi_k$. Then the distribution of value v_k has the form

$$\rho(|v_k|) = \frac{1}{b|v_k|}, \quad \omega_0 < |v_k| < \omega_1. \tag{19}$$

The frequency distribution density (18) can be determined as

$$\rho_{\text{qlv}}(\omega) = \frac{d}{d\omega} P(|v_k| < \omega)^{2n}, \tag{20}$$

where $P(|v_k| < \omega)$ is the probability to encounter element v_k, the modulus of which is smaller than ω. This probability for distribution (19) has the form

$$P(|v_k| < \omega) = \frac{1}{b} \ln \frac{\omega}{\omega_0}. \tag{21}$$

The obtained distribution can be written as a power-series distribution of frequency logarithm $\Lambda = \ln(\omega/\omega_0)$:

$$\rho_{\text{qlv}}(\Lambda) = \frac{2n}{b^{2n}} \Lambda^{2n-1}. \tag{22}$$

The corresponding frequency distribution can be approximately considered to be a power one in the region of $\omega \sim c$, which is of the greatest interest

$$\rho_{\text{qlv}}(\omega) \sim \omega^{\frac{4n-2}{b}-1}. \tag{23}$$

The obtained result (23) in Fig. 2 is compared with the numerical calculation of density of states $\rho(\omega)$. It can be seen that the number of quasi-local vibrations increases with increasing non-Gaussian parameter b. Thereat, if non-Gaussianity is strong $b \gg 1$, an additional dependence $\rho_{\text{qlv}}(\omega) \propto \omega^{\gamma}$ arises with power $\gamma \approx (4n-2)/b - 1$. This result agrees with the numerical calculation result and is marked by a dashed line in Fig. 2. The coefficient at power dependence (23) goes beyond the used approximation (18), so the coefficient was fitted when plotting the dashed lines.

5. Discussion

In the present paper we have analyzed the distribution of quasi-local modes in the model of correlated random matrices. The distribution density at low frequencies is proportional to ω^n both for the Gaussian and for non-Gaussian distribution of the elements of the matrix $\hat{A}$. At the same time, for a large value of non-Gaussian the parameter b, a frequency range appears, at which the distribution density is proportional to ω^γ, where power γ depends both on the number of neighbors and on non-Gaussianity the parameter b. It can be considered that the parameter b reduces the effective number of the nearest neighbors to value γ. Indeed, many elements v_k for a strongly non-Gaussian distribution have a relatively small value and only the largest of them make a contribution to the quasi-local vibration frequency. The value of $\gamma \approx 4$, observed in many model glasses, can also be reproduced in the given model ($b = 4.4$ at $n = 6$). However, the statistics of the matrix elements is determined by many factors which takes place under cooling of model systems and obtaining of a stable atom configuration. A conclusion that $\gamma \approx 4$ is the effective number of neighboring atoms from the viewpoint of statistical properties of the matrix $\hat{A}$ can be made within the framework of the present paper, which takes into account the fundamental statistical properties (system stability and sum rule).

An important aspect is the spatial distribution of vibrations. The studied system contains phonons, the minimum frequency of which is determined by system elasticity and size. For instance, the lowest-frequency phonon in Fig. 1 at $\varkappa = 0.4$ is shaped as a peak at the frequency of $\omega \approx 0.35$. All lower-frequency vibrations are quasi-local are concentrated near an atom with index l, which corresponds to a soft mode.

In the present paper we have performed an analysis in a scalar vibration model, where it is considered (for simplicity) that the displacements of each atom from the equilibrium position is described by a scalar quantity. Consideration of the vector nature of vibrations complicates the analysis of the obtained results. Thereat, the main contribution to the spread in matrix elements is made by fluctuations of interatomic distances, since the force constants most significantly depend on the interatomic distance, which serves as a manifestation of the non-Gaussian statistics of matrix elements. Thus, the main conclusions in the present paper are also applicable to the vector model, in particular, for a strongly non-Gaussian distribution of matrix elements.

6. Conclusion

In the present paper the vibration peculiarities of soft regions in disordered systems are studied using the theory of correlated random matrices. It has been shown that the quantity and properties of such regions are considerably affected by the statistics of distribution of non-zero elements in the correlated the matrix $\hat{A}$. For this, we have found and studied the density of distribution of quasi-local vibrations $\rho_{\text{qlv}}(\omega)$, which corresponds to the low-frequency spectral region in the case of small system sizes.

The result of the found expressions for $\rho_{\text{qlv}}(\omega)$ is that the lowest-frequency region of vibrational states is described by dependence $\rho_{\text{qlv}}(\omega) \propto \omega^n$, where power n is the number of neighboring atoms. This result agrees with the results of the numerical calculation of the density of states for the entire system $\rho(\omega)$, for Gaussian and non-Gaussian statistics of matrix elements.

When the non-Gaussian the parameter b increases, the number of quasi-local vibrations also increases. An analysis of the vibrational state density has shown that the intermediate dependence $\rho_{\text{qlv}}(\omega) \propto \omega^\gamma$ arises in this case. This result makes it possible to describe the generally accepted dependence $\rho_{\text{qlv}}(\omega) \propto \omega^4$, observed in many amorphous systems [7,12,13]. This indicates that the model of random correlated matrices can be used to describe vibrations of soft regions of amorphous dielectrics.

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Conflict of interest

The authors declare that they have no conflict of interest.

Appendix 1

The problem of finding the distribution of the following quantity arises when studying the distribution of quasi-local vibration frequency

$$\omega = \sqrt{\xi \hat{C} \xi^T}, \tag{24}$$

where $\xi = (\xi_1, \ldots, \xi_{n+1})$ is the row vector of random numbers, and the matrix $\hat{C}$ is a positively defined symmetric matrix. The value of ξ_k has a distribution ρ_k.

We will solve this problem by decomposing the matrix $\hat{C}$ in eigenvalues

$$\hat{C} = \hat{U} \hat{D} \hat{U}^T, \tag{25}$$

where $\hat{U}$ is an orthogonal matrix, while diagonal the matrix $\hat{D}$ is composed of eigenvalues of the matrix $\hat{C}$: $\lambda_c = \lambda_1, \ldots, \lambda_{n+1}$, $\lambda_k > 0$. Then

$$\omega = \sqrt{\sum_{k=1}^{n+1} \lambda_k y_k^2}, \tag{26}$$

where value $y_k = \sum_{m=1}^{n+1} U_{km} \xi_m$.

The probability that random value (26) is lower than a certain preset small number W is determined by the volume of a $(n+1)$--dimensional ball

$$P(\omega < W) = \frac{\pi^{\frac{n+1}{2}} W^{n+1}}{\Gamma\left(\frac{n+1}{2}+1\right)} \prod_{k=1}^{n+1} \lambda_k^{-1/2} h_k(0), \qquad (27)$$

where h_k is distribution density y_k.

We will use the fact that distribution density at the origin of coordinates $y = \xi = 0$ does not change upon a n-dimensional turn $y = \hat{U}\xi$. Moreover, the product of all eigenvalues sets a matrix determinant: $\prod_{k=1}^{n+1} \lambda_k = \det \hat{C}$. Therefore, distribution density $\rho(\omega)$, averaged over different implementations of the matrix $\hat{C}$, at small values $\omega \ll 1$ has the following form:

$$\rho(\omega) = \frac{2\pi^{\frac{n+1}{2}} \omega^n}{\Gamma\left(\frac{n+1}{2}\right)} \left\langle \det(\hat{C})^{-1/2} \right\rangle \prod_{k=1}^{n+1} \rho_k(0). \qquad (28)$$

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