General behavior of the quenched averaged spectral density with a change in the ensemble probability distribution

M. Schulz
Fachbereich Physik, Technische Hochschule Merseburg, O-4200 Merseburg, Germany

K.Handrich
Fachbereich Physik, Technische Hochschule Ilmenau, O-7300 Ilmenau, Germany
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The behavior of the ensemble-averaged spectral density $\langle G(z)\rangle$ for a given eigenvalue problem $(z\delta_{ij}-\Phi_{ij})y_j=0$ with the random matrix $\mathbf{\Phi}$, distributed by the probability $P(\mathbf{\Phi})$, will be examined. By using the replica method, the change of $\langle G(z)\rangle$ for an infinitesimal neighboring distribution is calculated and, as a result, it was found that for systems with a higher disorder of the random matrix $\mathbf{\Phi}$ the averaged spectral density increases for very small and very large values of z, respectively.

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I. INTRODUCTION

For many physical problems, but also for other natural scientific and technical problems, the determination of the eigenvalue spectrum for an eigenequation

$$(z\delta_{ij}-\Phi_{ij})y_j=0, \tag{1}$$

in which $\mathbf{\Phi}$ is a symmetric $N\times N$ matrix, is a central question. For a sufficiently small N there exist well-known analytical and numerical methods for the solution of (1). For large N an analytical solution of (1) is possible in few cases (see, for example, the exact solution of the eigenvalue spectrum for an oscillator in quantum mechanics), but for many cases there is only a numerical solution [1,2] with a sufficiently small margin of error. To characterize the spectra of eigenvalues it is reasonable to use the spectral density

$$G(z)=\sum_{i=1}^{N}\delta(z-\lambda_i) \tag{2}$$

(λ_i, $i=1,\ldots,N$) is the set of the eigenvalues of Eq. (1). For many statistical problems the matrix $\mathbf{\Phi}$ is a stochastic object, which is realized with the probability distribution $P(\mathbf{\Phi})$. This distribution can be very complicated; for example, in the theory of lattice dynamics, in which $\mathbf{\Phi}$ is the dynamic matrix [3], the function P must guarantee that $\mathbf{\Phi}$ is always a positive-definite matrix.

In such cases it is of interest, from a physical point of view, to determine the average spectral density of (1). The average is performed over an ensemble of matrices $\mathbf{\Phi}$, which are distributed with the probability distribution $P(\mathbf{\Phi})$. Formally Eq. (1) can transformed into

$$(z\delta_{ij}-\langle\Phi_{ij}\rangle-\Delta\Phi_{ij})y_j=0, \tag{3}$$

in which $\langle\mathbf{\Phi}\rangle$ is the ensemble average of $\mathbf{\Phi}$, and $\Delta\mathbf{\Phi}$ is the deviation of the actual values from the averages ones. By analogy to the perturbation theory $\langle\mathbf{\Phi}\rangle$ is defined to be the undisturbed reference matrix and $(z-\langle\mathbf{\Phi}\rangle)\mathbf{y}=0$ is the undisturbed reference eigenvalue problem, whereas $\Delta\mathbf{\Phi}$ is the perturbation of the reference problem (with $\langle\Delta\mathbf{\Phi}\rangle=0$). The determination of the ensemble-averaged spectral density by numerical methods [4,5] is possible at a high expense of computation time and computer memory and only for relatively simple distributions $P(\mathbf{\Phi})$. Analytical methods exist for special Gauss-distributed matrices [6], and solutions, based on the perturbation theory, are possible for small deviations $\Delta\mathbf{\Phi}$ [7].

The aim of the following calculations is the determination of general information concerning the behavior of the averaged spectral density by a change of the probability distribution $P(\mathbf{\Phi})$ under the restriction that all $P(\mathbf{\Phi})$ generate the same average $\langle\mathbf{\Phi}\rangle$, e.g., the same reference problem. Using general thermodynamical methods for excitations in an amorphous system it is possible to show [8] that with a higher disorder of the amorphous solid the averaged spectral density increases in the region $z=\omega^2\to z_{\min}=0$. We will give a proof that such an increase at an end point of a spectrum $z_{\min}$ or $z_{\max}$ [e.g., all eigenvalues of each possible matrix with nonvanishing probability $P(\mathbf{\Phi})$ are contained in the region $z>z_{\min}$ and $z<z_{\max}$, respectively] is a general behavior.

II. GAUSSIAN-GENERATED DISTRIBUTION FUNCTIONS

In a first step it is necessary to define a class of distribution functions, which are reasonably called as infinitesimal Gaussian-generated functions: If two infinitesimal neighboring probability distributions $P(\mathbf{\Phi})$ and $P'(\mathbf{\Phi})$ are connected by the relation

$$P'(\mathbf{\Phi}) = \int D[\Phi']P(\mathbf{\Phi}')\mathcal{N}(\mathbf{\Phi}') \times \exp\left(-(\Phi'_{ij} - \Phi_{ij})\frac{m(\mathbf{\Phi}')_{ijkl}}{\sigma}(\Phi'_{kl} - \Phi_{kl})\right), \tag{4}$$

in which $\mathcal{N} = (\det \mathbf{m})^{1/2}$ is the norm constant, σ is an infinitesimal positive scalar value, and $m(\mathbf{\Phi})$ a symmetric and positive-definite tensor function, e.g.,

$$m(\mathbf{\Phi})_{ijkl} = m(\mathbf{\Phi})_{klij} \tag{5}$$

and

$$m(\mathbf{\Phi})_{ijkl}\alpha_{ij}\alpha_{kl} > 0 \tag{6}$$

for an arbitrary matrix α, then the probability distribution $P'(\mathbf{\Phi})$ is called an infinitesimal Gaussian generation from $P(\mathbf{\Phi})$.

Note that because of the symmetry of the matrix $\mathbf{\Phi}$, it follows that

$$m(\mathbf{\Phi})_{ijkl} = m(\mathbf{\Phi})_{jikl} = m(\mathbf{\Phi})_{ijlk} = \cdots . \tag{7}$$

Principally there is the possibility, starting by a probability distribution $P_0(\mathbf{\Phi})$, to generate new probability distributions, which are the basis for the next Gaussian generation and so on. In this way a tree (network) of Gaussian generated distribution functions can be obtained, which are based on the same root P_0. It is simple to show that, because of (4), the ensemble average $\langle\mathbf{\Phi}\rangle$ is a conservation value for the given network. Moreover, it can be shown that the variance of

$$\mathrm{var}_{ijkl}(\mathbf{\Phi}) = \langle\Phi_{ij}\Phi_{kl}\rangle - \langle\Phi_{ij}\rangle\langle\Phi_{kl}\rangle \tag{8}$$

increases under an infinitesimal Gaussian generation. (Note that it is reasonable to use the norm $\mid \mathrm{var}(\mathbf{\Phi}) \mid = \sup[\mathrm{var}(\mathbf{\Phi})\alpha_{ij}\alpha_{kl} \mid \alpha \mid^{-2}]$ as a measure for the strength of the variance.) We get

$$\mathrm{var}(\mathbf{\Phi})' = \mathrm{var}(\mathbf{\Phi}) + \sigma \int D\Phi P(\mathbf{\Phi})\mu_{ijkl}(\mathbf{\Phi}) \tag{9}$$

(μ is the inverse value of $\mathbf{m}$, e.g., $m_{ijmn}\mu_{mnkl} = \delta_{ik}\delta_{jl}$) for an infinitesimal Gaussian generation. The difference $\delta P(\mathbf{\Phi}) = P'(\mathbf{\Phi}) - P(\mathbf{\Phi})$ between functional neighboring probability distributions, which are connected by an infinitesimal Gaussian generation, can be written by using the Fourier representation as

$$\delta P(\mathbf{\Phi}) = \int D\Phi\, D\left[\frac{k}{2\pi}\right] P(\mathbf{\Phi}')\exp\{ik_{ij}(\Phi'_{ij} - \Phi_{ij})\} \times[\exp\{-\tfrac{1}{4}\sigma\mu_{ijkl}(\mathbf{\Phi}')k_{ij}k_{kl}\} - 1] = -\frac{\sigma}{4}\frac{\partial}{\partial\Phi_{ij}}\frac{\partial}{\partial\Phi_{kl}}\left[\mu_{ijkl}(\mathbf{\Phi})P(\mathbf{\Phi})\right]. \tag{10}$$

Clearly, the inverse infinitesimal Gaussian generation $P' \to P$ is determined by the opposite sign. Hence an arbitrary transformation between two infinitesimal neighboring probability distributions $P \to P''$ can be represented by an infinitesimal Gaussian generation $P \to P'$ and an inverse infinitesimal Gaussian generation $P' \to P''$ with the difference

$$\delta P(\mathbf{\Phi}) = -\frac{\sigma}{4}\frac{\partial}{\partial\Phi_{ij}}\frac{\partial}{\partial\Phi_{kl}}\{[\mu^1_{ijkl}(\mathbf{\Phi}) - \mu^2_{ijkl}(\mathbf{\Phi})]P(\mathbf{\Phi})\}. \tag{11}$$

On the other hand, each tensor γ with the same symmetry properties as μ can be determined as a difference of two positive definite tensors μ^1 and μ^2; e.g., we get instead of (11)

$$\delta P(\mathbf{\Phi}) = -\frac{\sigma}{4}\frac{\partial}{\partial\Phi_{ij}}\frac{\partial}{\partial\Phi_{kl}}[\gamma_{ijkl}(\mathbf{\Phi})P(\mathbf{\Phi})]. \tag{12}$$

Therefore, the connection between two probability distributions $P_0(\mathbf{\Phi})$ and $P_e(\mathbf{\Phi})$, which are separated by an infinite set of different infinitesimal Gaussian generations and inverse Gaussian generations, can be described by the parabolic differential equation

$$\frac{\partial P(s,\mathbf{\Phi})}{\partial s} = -\frac{1}{4}\frac{\partial}{\partial\Phi_{ij}}\frac{\partial}{\partial\Phi_{kl}}[\gamma_{ijkl}(s,\mathbf{\Phi})P(s,\mathbf{\Phi})], \tag{13}$$

with the path parameter s and the boundary conditions $P_0(\mathbf{\Phi}) = P(s=0,\mathbf{\Phi})$ and $P_e(\mathbf{\Phi}) = P(s=L,\mathbf{\Phi})$. On the other hand, it follows from (9) that the behavior of the variance $\mathrm{var}(\mathbf{\Phi})$ is determined by the equation

$$\mathrm{var}(\mathbf{\Psi})\mid_e - \mathrm{var}(\mathbf{\Psi})\mid_0 = \int_0^L ds \int D\Phi\, P(s,\mathbf{\Phi})\gamma_{ijkl}(s,\mathbf{\Phi}). \tag{14}$$

III. CHANGE OF SPECTRAL DENSITY

Now we will examine in what respect the ensemble-average spectral density $\langle G(z)\rangle$ changes its functional structure by a transition between two infinitesimal neighboring probability distributions P and P', which are connected by a Gaussian generation (4). We use the following representation [6] for the spectral density:

$$G(z,\mathbf{\Phi}) = \frac{2}{\pi}\lim_{\epsilon\to 0}\frac{\partial}{\partial z}\mathrm{Im}\,\ln Z. \tag{15}$$

Here

$$Z = \int Dx \exp\{i(z\delta_{ij} + i\epsilon\delta_{ij} - \Phi_{ij})x_i x_j\}. \tag{16}$$

Using the expression (4), the ensemble average of $\langle G(z)\rangle'$ for the probability distribution P' is given by

$$\begin{aligned}\langle G(z)\rangle' &= \int D\Phi\; G(z,\mathbf{\Phi})P'(\mathbf{\Phi})\\ &= \int D\Phi' D\xi\; P(\mathbf{\Phi}')G(z,\mathbf{\Phi}'+\xi)N(\mathbf{\Phi}')e^{-\xi_{ij}[m_{ijkl}(\mathbf{\Phi}')/\sigma]\xi_{kl}}\\ &= \int D\Phi'\; P(\mathbf{\Phi}')\overline{G(z,\mathbf{\Phi}'+\xi)}. \end{aligned} \tag{17}$$

In this expression the average $\overline{G(z,\mathbf{\Phi}'+\xi)}$ is the Gaussian average (determined by $\mathbf{m}$ and σ over the difference value $\xi=\mathbf{\Phi}-\mathbf{\Phi}'$ for an arbitrary, but fixed state $\mathbf{\Phi}'$). For the following calculations the replica trick [9,10]

$$\ln Z = \lim_{n\to 0}\frac{Z^n-1}{n} \tag{18}$$

was used. Thus with (15), 16), and (18) the Gaussian averaged value $\overline{G(z,\mathbf{\Phi}'+\xi)}$ becomes

$$\overline{G(z,\mathbf{\Phi}'+\xi)} = \frac{2}{\pi}\lim_{\epsilon\to 0}\lim_{n\to 0}\frac{1}{n}\mathrm{Im}\frac{\partial}{\partial z}\int DxD\xi\exp\left\{\frac{i}{2}\sum_{\alpha=1}^{n}\left[(z\delta_{ij}+i\epsilon\delta_{ij}-\Phi'_{ij}-\xi_{ij})x_i^\alpha x_j^\alpha-\xi_{ij}\frac{m_{ijkl}(\mathbf{\Phi}')}{\sigma}\xi_{kl}\right]\right\}. \tag{19}$$

After a rotation of the coordinate system (in such a way that $\mathbf{\Phi}'$ becomes a diagonal matrix $\lambda_i\delta_{ij}$) $\mathbf{x}\to\tilde{\mathbf{x}}$, with $\xi\to\tilde{\xi}$, $\mathbf{\Phi}'\to\tilde{\mathbf{\Phi}}'$, $\mathbf{m}(\mathbf{\Phi}')\to\tilde{\mathbf{m}}(\tilde{\mathbf{\Phi}}')$ [$\tilde{\mathbf{m}}(\tilde{\mathbf{\Phi}}')$ fulfills the same demands as $\mathbf{m}(\mathbf{\Phi}')$], and the integration over the $\tilde{\xi}$, we get

$$\overline{G(z,\mathbf{\Phi}'+\xi)} = \frac{2}{\pi}\lim_{\epsilon\to 0}\lim_{n\to 0}\frac{1}{n}\mathrm{Im}\frac{\partial}{\partial z}\int D\tilde{x}\exp\left\{\frac{i}{2}\sum_{\alpha=1}^{n}\sum_{i=1}^{N}(z+i\epsilon-\lambda_i)(\tilde{x}_i^\alpha)^2-\frac{\sigma}{4}\sum_{\alpha,\beta}\tilde{x}_i^\alpha\tilde{x}_j^\alpha\tilde{\mu}_{ijkl}(\tilde{\mathbf{\Phi}}')\tilde{x}_k^\beta\tilde{x}_l^\beta\right\} \tag{20}$$

[$\tilde{\mu}(\tilde{\mathbf{\Phi}}')$ is the inverse tensor of $\tilde{\mathbf{m}}(\tilde{\mathbf{\Phi}}')$]. The Taylor expansion of $\overline{G(z,\mathbf{\Phi}'+\xi)}$ gives, in the lowest order of σ,

$$\overline{G(z,\mathbf{\Phi}'+\xi)} = G(z,\mathbf{\Phi}')+\sigma\left[\frac{\partial}{\partial\sigma}\overline{G(z,\mathbf{\Phi}'+\xi)}\,|_{\sigma=0}\right]. \tag{21}$$

The differential quotient in (21) follows from (20) by a simple integration over $\tilde{x}$, e.g.,

$$\begin{aligned}\frac{\partial}{\partial\sigma}\overline{G(z,\mathbf{\Phi}'+\xi)}\,|_{\sigma=0} = \frac{1}{2\pi}\lim_{\epsilon\to 0}\lim_{n\to 0}\frac{1}{n}\frac{\partial}{\partial z}\mathrm{Im}\prod_{k=1}^{N}\left(\frac{i\pi}{z+i\epsilon-\lambda_k}\right)^{n/2}\\ \times\sum_{\alpha,\beta}\sum_{i,j}\frac{1}{(z+i\epsilon-\lambda_i)(z+i\epsilon-\lambda_j)}\\ \times[\tilde{\mu}_{ijji}(\tilde{\mathbf{\Phi}}')(\delta_{\alpha\beta})^2+\tilde{\mu}_{ijij}(\tilde{\mathbf{\Phi}}')(\delta_{\alpha\beta})^2+\tilde{\mu}_{iijj}(\tilde{\mathbf{\Phi}}')\delta_{\alpha\alpha}\delta_{\beta\beta}]. \end{aligned}\tag{22}$$

Using the symmetry relations (7), which also apply for $\tilde{\mu}_{ijkl}$, it follows that

$$\begin{aligned}\overline{G(z,\mathbf{\Phi}'+\xi)}\,|_{\sigma=0} &= \frac{1}{2\pi}\lim_{\epsilon\to 0}\lim_{n\to 0}\frac{1}{n}\frac{\partial}{\partial z}\mathrm{Im}\prod_{k=1}^{N}\left(\frac{i\pi}{z+i\epsilon-\lambda_k}\right)^{n/2}\\ &\quad\times\sum_{i,j}\frac{1}{(z+i\epsilon-\lambda_i)(z+i\epsilon-\lambda_j)}[2\tilde{\mu}_{ijij}(\tilde{\mathbf{\Phi}}')n+\tilde{\mu}_{iijj}(\tilde{\mathbf{\Phi}}')n^2]\\ &= \frac{1}{\pi}\lim_{\epsilon\to 0}\frac{\partial}{\partial z}\mathrm{Im}\sum_{i,j}\frac{\tilde{\mu}_{ijji}}{(z+i\epsilon-\lambda_i)(z+i\epsilon-\lambda_j)}. \end{aligned}\tag{23}$$

For the following interpretation we integrate this value and get

$$h(y,\mathbf{\Phi}') = \int_{-\infty}^{y}dz'\int_{-\infty}^{z'}dz\overline{G(z,\mathbf{\Phi}'+\xi)}\,|_{\sigma=0}, \tag{24}$$

with

$$h(y,\mathbf{\Phi}') = 2\sum_{\substack{i,j\\ i\neq j}}\Theta(y-\lambda_i)\Theta(\lambda_j-y)\frac{\tilde{\mu}_{ijij}}{\lambda_j-\lambda_i} + \sum_i\tilde{\mu}_{iiii}\delta(y-\lambda_i). \tag{25}$$

Note that because $\tilde{\mu}$ is positive definite the diagonal elements $\tilde{\mu}_{ijij}$ are always positive, e.g., $h(y,\mathbf{\Phi}')$ is for all values y a positive value. With the definition

$$H(y) = \int_{-\infty}^{y}dz'\int_{-\infty}^{z'}dz\langle G(z)\rangle, \tag{26}$$

(17), and (21), it follows that

$$\delta H(y) = H'(y)-H(y) = \sigma\int D\Phi' P(\mathbf{\Phi}')h(y,\mathbf{\Phi}'). \tag{27}$$

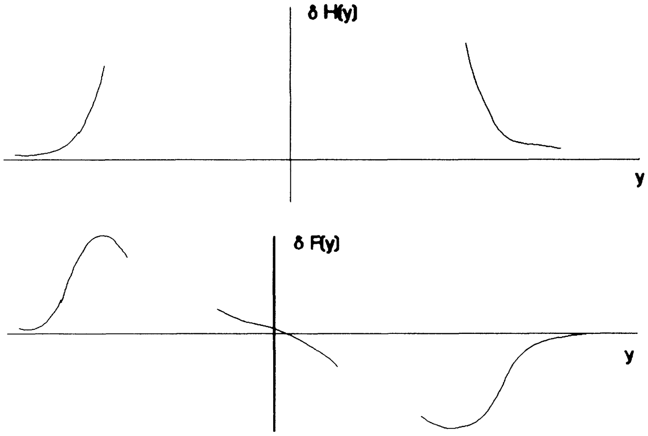

FIG. 1. The general structure of $\delta H(y)$ and $\delta F(y) = dH(y)/dy$.

Therefore, the correcture of $H(y)$ after an infinitesimal Gaussian generation is always positive (Fig. 1)

The differential quotient

$$F(y) = \frac{dH(y)}{dy} \tag{28}$$

is the number of states whose eigenvalues are smaller than y, e.g.,

$$\delta F(y) = \frac{d\delta H(y)}{dy} \tag{29}$$

is the change of this number of states in the course of the infinitesimal Gaussian generation. From Fig. 1 it is simple to construct the general structure of $\delta F(y)$. The differential quotient $\delta F(y)$ is a positive value for very small values y and a negative value for very large values y. Therefore it follows that $\delta F(y)$ has at least one point with $\delta F(y) = 0$.

The differentiation of $\delta F(z) = 0$ with respect to z gives the difference between the two neighboring averaged spectral densities

$$\delta \langle G(z) \rangle = \langle G(z) \rangle' - \langle G(z) \rangle = \frac{d\delta F(z)}{dz}. \tag{30}$$

This difference is positive for very small and very large values of y and negative for at least one interval between these two regions (see Fig. 2).

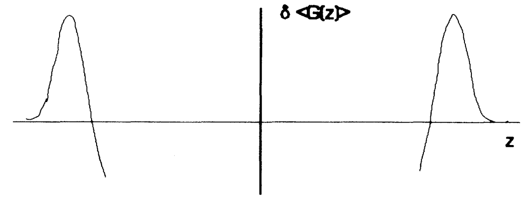

FIG. 2. The general structure of the function $\delta\langle G(z)\rangle$.

IV. DISCUSSION AND CONCLUSIONS

For a combination of an infinitesimal Gaussian generation and an inverse infinitesimal Gaussian generation we get the same result (25), but the positive-definite tensor $\tilde{\mu}$ must be replaced by the general tensor $\tilde{\gamma}$ with the same symmetric properties as $\tilde{\mu}$.

In Sec. II it was shown that a transition between two infinitesimal neighboring probability distributions with the same average $\langle \phi \rangle$ is possible by using a path on the network of infinitesimal Gaussian generations. In the same way it is possible to find a path with an infinite number of steps between two arbitrary probability functions P_0 and P_e (with constant average $\langle \Psi \rangle$) as a solution of (13). For a path $P_0 \rightarrow P_e$, which exclusively consists of Gaussian generations, it is clear that the change of the ensemble-averaged spectral density has the same general behavior as the change by one Gaussian generation. Analogically, it can be expected that for a path with predominant Gaussian generations and only a few inverse Gaussian generations, the ensemble-averaged spectral density shows with a high probability the same structural changes. In this case the norm $\mid \mathrm{var}(\mathbf{\Phi}) \mid$ of the variance increases by a transition from P_0 to P_e. Therefore, the change of this norm is a reasonable parameter for the characterization of the change of the spectral density. Clearly, for a path $P_0 \rightarrow P_e$, which consists of inverse Gaussian generations (exclusive or predominant) the inverted general behavior follows for the change of $\langle G(z) \rangle$ as in the cases discussed above. Here a similar decrease of $\mid \mathrm{var}(\mathbf{\Phi}) \mid$ is expected. If the path $P_0 \rightarrow P_e$ is constructed by Gaussian generations and inverse Gaussian generations with approximately equal portions, then it is not always possible to give a concrete assertion on the change of the ensemble-averaged spectral density. In this case the behavior of the norm $\mid \mathrm{var}(\mathbf{\Phi}) \mid$ and $\langle G(z) \rangle$ is also indeterminate and it must be calculated for each special case by us in Eqs. (13), (14), and (25)–(30).

[1] G. Jacucci, M.L. Klein, and R. Taylor, Phys. Rev. B **18**, 3782 (1978).

[2] T. Schneider and E. Stoll, Phys. Rev. B **17**, 1302 (1978); **18**, 6968 (1978).

[3] H. Böttger, *Principles of the Theory of Lattice Dynamics* (Akademie-Verlag, Berlin, 1983).

[4] D. Beeman and R. Alben, Adv. Phys. **26**, 339 (1977).

[5] F. Abraham, Adv. Phys. **35**, 1 (1986).

[6] S.F. Edwards and R.C. Jones, J. Phys. A **10**, 1595 (1976).

[7] I.M. Lifshits, S.A. Gredeskul, and L.A. Pastur, *Introduction to the Theory of Disordered Systems* (Wiley, New York, 1988).

[8] K. Handrich, Zh. Eksp. Teor. Fiz. **37**, 1383 (1973) [Sov. Phys. JETP **64**, 703 (1973)].

[9] S.F. Edwards *Proceedings of the Fourth Conference on Amorphous Materials*, edited by R.W. Douglas and B. Ellis (Wiley, New York, 1973).

[10] S.F. Edwards and P.W. Anderson, J. Phys. F **5**, 965 (1975).