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General description of homogeneous isotropic disordered systems

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Résumé . — Considérant que toutes les grandeurs physiques utiles à la description d'un tel système sont des tenseurs sphériques, il est démontré que les hypothèses d'homogénéité et d'isotropie statistiques imposent à leurs fonctions de corrélation spatiales croisées de telles contraintes que ces dernières s'expriment à l'aide de quelques fonctions scalaires véhiculant toute l'information et de fonctions sphériques standard. Les deux limites d'un système perturbé par beaucoup de défauts indépendants, entraînant une statistique de Gauss, ou d'un assemblage de microcristaux, plus analogue à une distribution de Poisson, sont présentées.

Abstract . — As all the physical quantities describing such a system are spherical tensors, it is shown that homogeneity and isotropy imply for the cross-correlation functions such conditions that they can be written with only standard spherical functions and a few scalar functions in which the whole physical information is included. The two limiting cases of a system with many independent defects and of a polycrystal, Gauss and Poisson limits, are discussed.

1. Introduction.

There is a strong analogy between the statistical description of a disordered system, even a static one, and a random process. In the last case, one or several variables are assumed to be time dependent, and the way they vary with time changes from one experiment to another. As one is interested in the permanent characteristic features of the processes, one takes mean values, even mean values of fluctuations and, in the case of ergodicity, one can in principle compute any physical quantity to be compared with measurements.

In the case of a disordered system, one assumes the random event not to be the time of the experiment, but the choice of the sample, and one hopes enough reproducibility from one sample to another for making a kind of space ergodicity hypothesis. But one has no more a random function but a random field and one must go to a new order of complexity. If the

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field one is interested in is a tensorial one, one may even have difficulties in trying to imagine simple pictures.

It is true that many situations are well described by uncorrelated fields, that is by assuming that the parameters vary independently on each atomic site. This is enough to describe weak localization [1], spin glasses [2], many magnetic properties [3], but the presence of correlations between the values of the fields at different sites may alter phenomena, or even change the qualitative picture of them; this concerns every effect where a length characteristic of the phenomenon is to be compared with the correlation length of the disorder itself. As examples, let us mention quantum localization [4], depolarization of light in liquids [5], in solids [6], of neutrons in disordered magnets [7] and even the magnetostatic behavior of those materials [8]. So one needs a more complete formalism, which has been developed mainly for scalar fields [6].

There is nevertheless a case where one can go far enough, it is the situation where one has both statistical homogeneity and statistical isotropy. Here, the mean values we shall have to consider will be both translation and rotation invariant, and those properties will simplify their expressions, exactly for the same reasons group theory is an important tool in atomic physics. The purpose of this note is to present the main features of those simplifications, and after having shown the effects of rotation invariance, then of translation homogeneity, to present two limiting cases, similar in the case of disordered systems, to the Gauss and Poisson limits for random time processes.

2. The effect of rotational invariance.

Let us assume that, in each point, the physics is described through several tensorial parameters which can always be reduced to spherical tensors [10]. When the reference axis rotates, if R denotes the rotation matrix

$$x'_i = \sum_j R_{ij} x_j,$$

the components of a spherical tensor are changed following the law

$$T_{lm}(\mathbf{r}) = \sum_{m'} T_{lm'}(R\mathbf{r}) \mathcal{D}_{m'm}^l(R) \quad (1)$$

where l is the order of the tensor, m and m' run over the $(2l+1)$ values from $-l$ to l , and $\mathcal{D}^l(R)$ is the standard matrix of the l^{th} representation of the rotation group.

The correlation between two different spherical tensors is given by

$$G_{ll'mm'}(\rho; TT') = \langle T_{lm}(\mathbf{r} + \rho) T_{l'm'}'(\mathbf{r}) \rangle \quad (2)$$

where the brackets designate a statistical mean, which is independent of $\mathbf{r}$, due to the space ergodicity hypothesis.

The $G_{ll'mm'}(\rho; TT')$ depend not only of ρ , but also of the axis orientation; the indices m and m' are here to remind us that one has already chosen at least a z direction. There is no loss of generality in writing the dependence on ρ as a function of $\rho = |\rho|$ multiplied by spherical harmonics $Y_{LM}(\rho)$, where only the angles of the vector with the coordinate axis are arguments of the spherical functions. This is

$$G_{ll'mm'}(\rho; TT') = \sum_{LM} G_{ll'mm'LM}(\rho; TT') Y_{LM}(\rho) \quad (3)$$

One can now rotate the coordinate axis, and apply (2) and (3) on one side, the rotation formula analogous to (1) for spherical harmonics to (3) on the other side. This gives

$$\begin{aligned} G_{ll'm_1m'_1}(\rho; TT') &= \sum_{LMM'} G_{ll'm_1m'_1LM}(\rho; TT') Y_{LM}(R\rho) \mathcal{D}_{M'M}^L(R) \\ &= \sum_{m_2m'_2L_2M_2} G_{ll'm_2m'_2L_2M_2}(\rho; TT') Y_{L_2M_2}(R\rho) \mathcal{D}_{m_2m_1}^l(R) \mathcal{D}_{m'_2m'_1}^{l'}(R) \end{aligned} \quad (4)$$

Here the isotropy hypotheses have already been made, when the same G function of ρ and of six indices has been used in the two lines. As the angular dependence of (4) is only in the Y_{LM} which form a complete basis over the ρ or the $R\rho$ directions, (4) can be written

$$\begin{aligned} \sum_M G_{ll'm_1m'_1LM}(\rho; TT') \mathcal{D}_{M'M}^L(R) &= \\ = \sum_{m_2m'_2} G_{ll'm_2m'_2LM}(\rho; TT') \mathcal{D}_{m_2m_1}^l(R) \mathcal{D}_{m'_2m'_1}^{l'}(R) \end{aligned} \quad (5)$$

In the theory of rotation group representations, one shows that

$$\mathcal{D}_{m_2m_1}^l(R) \mathcal{D}_{m'_2m'_1}^{l'}(R) = \sum_{\lambda\mu_2\mu_1} \langle lm_2l'm'_2 | ll'\lambda\mu_2 \rangle \mathcal{D}^{\lambda\mu_2\mu_1}(R) \langle ll'\lambda\mu_1 | lm_1l'm'_1 \rangle \quad (6)$$

where the summations over μ_1 and μ_2 are virtual due to the Σm conserving properties of the Clebsch-Gordan coefficients.

Introducing (6) into (5) and using the orthogonality properties of the $\mathcal{D}^l$ matrix elements over the Euler angles describing the rotations, one gets

$$\begin{aligned} G_{ll'm_1m'_1LM}(\rho; TT') &= \\ = \sum_{m_2m'_2} G_{ll'm_2m'_2LM}(\rho; TT') \langle lm_2l'm'_2 | ll'LM' \rangle \langle ll'LM | lm_1l'm'_1 \rangle \end{aligned} \quad (7)$$

The only M dependence of the right member is through the second vector coupling coefficient, the M' dependence of the right hand side G and of the first coupling coefficient is a fallacious one, as M' must be equal to $m_2 + m'_2$. So one can write

$$G_{ll'mm'LM}(\rho; TT') = \Gamma_{ll'L}(\rho; TT') \langle ll'LM | lml'm' \rangle \quad (8)$$

and so one has shown that

$$\langle T_{lm}(\mathbf{r} + \rho) T_{l'm'}^{l'}(\mathbf{r}) \rangle = \sum_L \langle lml'm' | ll'LM \rangle \Gamma_{ll'L}(\rho; TT') Y_{LM}(\rho) \quad (9)$$

It is easy to bring (9) into (7) and to check the coherence of this result, due to the unitary properties of the vector coupling Clebsch-Gordan coefficients.

3. The translational invariance.

A lot of simple properties of the Γ can be deduced. First of all, let us consider ρ as small and develop $G_{ll'mm'}(\rho; TT')$ in series of the components ρ_1, ρ_2, ρ_3 . The terms of each order can be regrouped in spherical tensors and it is clear that Y_{LM} cannot appear before order L . So for small ρ

$$\Gamma_{ll'L}(\rho; TT') = A_{ll'L}(TT')\rho^L + \dots \quad (10)$$

The addition rule for angular momenta fixes L to vary from $|l - l'|$ to $l + l'$. The $l = l'$ term is the only finite term for $\rho = 0$, so one has

$$\langle T_{lm}(\mathbf{r}) T'_{l'm'}(\mathbf{r}) \rangle = A_{ll'0}(TT') \langle l m l' m' | l l' 00 \rangle Y_{00}; \quad (11)$$

as

$$\langle l m l' m' | l l' 00 \rangle = \delta_{ll'} \delta_{m, -m'} \frac{(-1)^{l-m}}{\sqrt{2l+1}}$$

and

$$T_{l-m} = (-1)^m T_{lm}^*$$

it is better to write the local correlation function as

$$\langle T_{lm}(\mathbf{r}) T'_{l'm'}^*(\mathbf{r}) \rangle = \delta_{ll'} \delta_{mm'} \frac{\sigma_l^2(TT')}{2l+1} \quad (11)$$

One can define the correlation length $\rho_c(T)$ of a tensor field T , by writing $T' = T$ and

$$\int_0^\infty d\rho \langle T_{lm}(\mathbf{r} + \rho) T_{lm}^*(\mathbf{r}) \rangle = \rho_c(T) \sigma_l^2(T) \quad (12)$$

while other definitions are possible.

One can also Fourier transform the G s to get

$$G_{ll'mm'}(\rho; TT') = \int \frac{d^3\kappa}{8\pi^3} \exp(i\kappa \cdot \rho) G_{ll'mm'}(\kappa; TT') \quad (13)$$

The function $G(\kappa)$ can be analyzed as a sum of products of functions of $\kappa = |\kappa|$ by $Y_{LM}(\kappa)$, as was done in ρ space by (3).

Introducing

$$\exp(i\kappa \cdot \rho) = 4\pi \sum_{l=0}^{\infty} \sum_m i^l j_l(\kappa\rho) Y_{lm}^*(\kappa) Y_{lm}(\rho)$$

into (13), one gets

$$G_{ll'mm'L(m+m')}(\kappa; TT') = 4\pi i^{-L} \langle l m l' m' | l l' L(m+m') \rangle \int_0^\infty \rho^2 d\rho j_L(\kappa\rho) \Gamma_{ll'L}(\rho; TT') \quad (14)$$

where the j_L are spherical Bessel functions.

This Fourier transform can be done directly over the random variables $T_{lm}(\mathbf{r})$

$$T_{lm}(\mathbf{r}) = \int \frac{d^3\mathbf{k}}{8\pi^3} \exp(i\mathbf{k} \cdot \mathbf{r}) \tilde{T}_{lm}(\mathbf{k}) \quad (15)$$

and one can see immediately that

$$\begin{aligned}\langle \tilde{T}_{lm}(\mathbf{k}) \tilde{T}'_{l'm'}(\mathbf{k}') \rangle &= \int d^3\mathbf{r} d^3\mathbf{r}' \exp \{-i(\mathbf{k} \cdot \mathbf{r} + \mathbf{k}' \cdot \mathbf{r}')\} \langle T_{lm}(\mathbf{r}) T'_{l'mm'}(\mathbf{r}') \rangle \\ &= \int d^3\mathbf{r} d^3\mathbf{r}' \exp(-i\mathbf{k} \cdot \boldsymbol{\rho}) G_{ll'mm'}(\boldsymbol{\rho}; TT') \exp(-i(\mathbf{k} + \mathbf{k}') \cdot \mathbf{r}) \\ &= 8\pi^3 \delta(\mathbf{k} + \mathbf{k}') G_{ll'mm'}(\mathbf{k}; TT')\end{aligned}\quad (16)$$

where

$$\boldsymbol{\rho} = \mathbf{r} - \mathbf{r}'$$

One sees that the translational invariance has imposed the statistical independence of the components of the T belonging to different $\mathbf{k}$ vectors. If the second random field introduced in (15) had been written as a conjugate one, one condition would have had a factor $\delta(\mathbf{k} - \mathbf{k}')$.

This independence of random variables in reciprocal space is known for scalar random fields and T called a field with orthogonal increments [9]. It has a simple consequence for the correlation function. Let us now write $G_{ll'mm'}(\boldsymbol{\rho})$ as a function of the $T_{lm}(\mathbf{k})$ by introducing (15) into (2).

One gets

$$G_{ll'mm'}(\boldsymbol{\rho}; TT') = \int \frac{d^3\mathbf{k}}{8\pi^3} \exp(i\mathbf{k} \cdot \boldsymbol{\rho}) \langle \tilde{T}_{lm}(\mathbf{k}) \tilde{T}'_{l'm'}(-\mathbf{k}) \rangle \quad (17)$$

that is

$$G_{ll'mm'}(\mathbf{k}; TT') = \langle \tilde{T}_{lm}(\mathbf{k}) \tilde{T}'_{l'm'}(-\mathbf{k}) \rangle$$

which is generalization of the Wiener-Khinchin theorem [11].

4. Two limiting cases.

When one considers a random process, that is a random function of the time, two limiting cases are physically important. Let us speak of the field seen by an atom as a function of time. If there are many independent sources, such as the effects of other atoms, one has a Gaussian process, with the central-limit theorem. The other extreme case is the one of an atom in a gas, suffering scarcely random strong collisions, which gives a Poisson statistics.

Here we have analogous cases. Either the field is created by numerous sources, say defects, dispersed in a crystal and what is seen is the linear superposition of their effects; this is the Gaussian process. The other possibility is the case of a polycrystal: if one travels along any straight line, the situation does not vary except when meeting a grain boundary. We shall show that the correlation functions of spherical tensor fields may have different behavior in the two cases, and that it is not necessary to go to the characteristic functions, or to the characteristic functionals, to see the difference.

In the case of a Gaussian random field, one may imagine that the positions $\mathbf{r}_i$ of the sources and their orientations R_i are random independent variables. If the field one is interested in is of spherical order l , it is reasonable to assume the sources to be of order $(l-1)$ to take into account the effect of the direction $\mathbf{r} - \mathbf{r}_i$. This gives

$$\begin{aligned}T_{lm}(\mathbf{r}) &= T_{l-1, m_0}, \sum_{m'} \langle l-1, m', 1, m-m' | l-1, 1, l, m \rangle \sum_i \mathcal{D}_{m_0, m'}^{l-1}(R_i) \\ &Y_{l, m-m'}(\mathbf{r} - \mathbf{r}_i) f(|\mathbf{r} - \mathbf{r}_i|),\end{aligned}\quad (18)$$

where $f(|\mathbf{r} - \mathbf{r}_i|)$ describes the effect of the distance between source and observation point. As $\mathbf{r}_i$ and R_i are random, one has, using the properties of the spherical harmonics

$$\langle T_{lm}(\mathbf{r} + \boldsymbol{\rho}) T_{lm}(\mathbf{r})^* \rangle = |T_{l-1, m_0}|^2 \sum_i \frac{3}{4\pi} \cos[(\mathbf{r} + \boldsymbol{\rho} - \mathbf{r}_i) \cdot (\mathbf{r} - \mathbf{r}_i)] \\ f(|\mathbf{r} + \boldsymbol{\rho} - \mathbf{r}_i|) f(|\mathbf{r} - \mathbf{r}_i|)$$

Changing the variables and taking the mean values over a uniform repartition of the sources $\mathbf{r}_i$, neglecting their hard core interactions, one gets a behavior like

$$G_{ll'mm'}(\boldsymbol{\rho}; TT^*) \propto \int d^3\mathbf{r} (\mathbf{r} + 1/2\boldsymbol{\rho}) \cdot (\mathbf{r} - 1/2\boldsymbol{\rho}) f_1(|\mathbf{r} + 1/2\boldsymbol{\rho}|) f_1(|\mathbf{r} - 1/2\boldsymbol{\rho}|) \quad (19)$$

where

$$f_1(r) = r^{-1} f(r) \quad (20)$$

One sees that G decreases with distance following a power law, if the interaction function is such, that is if the interaction is mediated by a zero mass particle. In the case of an insulator with virtual excitation through the band gap, one will have an exponential decay with distance.

In the other case, a polycrystal, a possible model would be to take $\mathbf{r}_i$ for the centers of the grains, R_i for their orientations and to decide that the i^{th} grain is the region nearer $\mathbf{r}_i$ compared to every other $\mathbf{r}_j$ this gives

$$T_{lm}(\mathbf{r}) = T_{l, m_0} \left\langle \prod_{j \neq i} \eta[(2\mathbf{r} + \boldsymbol{\rho} - \mathbf{r}_i - \mathbf{r}_j) \cdot (\mathbf{r}_i - \mathbf{r}_j)] \eta[(2\mathbf{r} - \boldsymbol{\rho} - \mathbf{r}_i - \mathbf{r}_j) \cdot (\mathbf{r}_i - \mathbf{r}_j)] \right\rangle \quad (21)$$

and it is clear that before taking the mean values over the position $\mathbf{r}_i$ one single term is not zero, describing the fact that from one grain to another there is no correlation of orientation at all. Expression (21) can be evaluated in two ways, the first one by remarking that the condition that both points $\mathbf{r} + 1/2\boldsymbol{\rho}$, $\mathbf{r} - 1/2\boldsymbol{\rho}$ are on the same side of the mediatrix of the segment $\mathbf{r}_i$, $\mathbf{r}_j$ gives a factor

$$1 - \frac{|\boldsymbol{\rho} \cdot (\mathbf{r}_i - \mathbf{r}_j)|}{|\mathbf{r}_i - \mathbf{r}_j|^2},$$

and that for ρ small compared to $|\mathbf{r}_i - \mathbf{r}_j|$, the product of many such factors gives an exponential. But it is simpler to remark that when going along a straight line, the probability of having not yet met a boundary is proportional to

$$\exp \left\{ \frac{\alpha |\rho|}{\langle |\mathbf{r}_i - \mathbf{r}_j| \rangle} \right\}$$

where α is a numerical factor of the order of unity.

So one sees that in the case of the polycrystal the correlation function decreases exponentially with length, while in the Gaussian case the power law behavior is favored.

5. Conclusions.

We have shown that a generalization of the theory of random functions, a theory built for random time events, can be established to describe disordered solids, glasses or even fluctuations in liquids if one adds a time dependence. The fractal nature of the sets, where the modulus of such a random function - here a tensorial one - is larger than a given number, is also a simple property of the model, at least in the Gaussian limit; this property, which has been shown to be valid for scalar space functions [7] as well as for random noise [13], was pointed out to me by R. Rammal.

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