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Dynamic characteristics of the effective susceptibility function in random three-component system

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HIGHLIGHTS

- We apply renormalization method to obtain dynamic effective susceptibility of random three-component system.
- We explore effect of double-percolation for different combinations of static susceptibilities
- We explore the case when peculiarities of random three-component system are the most apparent.

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ABSTRACT

In this work we investigated dynamic characteristics of the effective susceptibility of random three-component system. We have shown that in the case of large discrepancy of the static local susceptibilities effective dynamic properties are similar to the two component system. If static coefficients of local dynamic susceptibilities of the components approach each other keeping relaxation parts different, then peculiarities of the three-component system become apparent. In this case the effective active part of the susceptibility possesses two plateaus and the relaxing part demonstrates two maximums. Amplitudes of the maximums for relaxing part depend on the dominating component.

Also we investigated a case of double percolation showing that the effective properties can change two times during variation of the fraction of one of the components. In the first case the change is associated with creation of the percolation cluster built from the component (2), the second change is linked to the extrusion of the component (2) and (3) by the component (1) which builds a secondary percolation cluster.

1. Introduction

Percolation theory [1,2] has applications in such various research fields as metal–insulator transitions [3,4], gelation processes [5], fluid flow in porous media [6], and viscoelasticity [7–9]. For the modeling of these diverse physical phenomena, as a rule every element of lattice representing a two-component system, is randomly assigned to be in one of two possible states. For example, in regular bond percolation, a bond is "black" with probability $p \in [0, 1]$ or "white" with probability $q = 1 - p$.

Zallen [10] generalized the conventional two-component percolation problem to a multi-component which he named polychromatic percolation and provided an in-depth study of its characteristics. Physical properties of polychromatic percolation were studied by Kogut and Straley [11] who applied dual lattice and Monte-Carlo approaches in the investigation of a bicritical exponent of conductivity. Later, Halley et al. [12] used finite-lattice simulations and effective medium theory to

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understand the conductivities of disordered lattices in which there were up to four species. Subsequently, Halley et al. [13] provided a general review of the work carried out so far on polychromatic percolation models. Developed mathematical tools have been successfully applied to explain experiments with hopping conductivity [14–17], polydisperse granular materials [18,19], sodium–ammonia mixtures and charge-transfer salts [12,13], high-temperature superconducting [20].

The motives for the current work are, first, to begin a systematic investigation of properties of effective *dynamic* susceptibility for the case of polychromatic percolation which can be expected ultimately to find a wide range of application in real multi-component systems of scientific and technical interest [21]. Second, we explore the idea of hierarchical averaging and renormalization in multi-component percolation and present results for a wide range of concentrations of constituent components.

In this work we will show that the effective dynamic susceptibility of the random three-component system is fundamentally different than for the case of the regular two-component system in several important respects. The difference can be explained from the point of view of microgeometry, namely, in three-component systems there are two interfaces analogous to the hull. In addition to the external surfaces, there are regions where all three components combine, affecting the dynamic of effective susceptibility properties.

Measuring effective dynamic susceptibility is widely used for characterizing highly disordered composite materials and based on relations between macroscopic properties and structure at the microscopic scale commensurate with the minimal length of the inhomogeneity. Establishing such relations remains a fundamental challenge due to lack of perturbation parameter. For the first time, we show that the effective dynamic susceptibility distinguishes between the composites with different fractions of components in a broadband frequency range. Our approach enables the interpretation of measurements by objectively selecting and modeling the most relevant features of parameters of constitutive components, and allows predicting properties of metamaterials.

2. Theory

2.1. A hierarchical model of composite consisting of three components

We consider composite as a three component random structure which can be mapped onto two-dimensional (*2D*) square lattice and investigated by percolation theory methods. Assume that each bond of the lattice is colored "black" with probability p, "white" with probability q, and "gray" with probability r, representing components of composite and satisfying the condition:

$$\begin{cases} p+q+r=1 \\ \tilde{D}\,(p,q,r) : 0 \le p \le 1;\ 0 \le q \le 1;\ 0 \le r \le 1, \end{cases} \tag{1}$$

where $\tilde{D}\,(p,q,r)$ is a probability domain. Geometrically $\tilde{D}\,(p,q,r)$ depicts an equiangular polygon (triangle) and probabilities p, q, and r can be interpreted as components of a vector. Of note, the regular two-component composite in Eq. (1) is recovered if either p, q, or r is zero.

Physical properties of such material can be described by the generalized ternary local probability density function:

$$\rho\left(G^*_{(km)}\right) = p\delta\left(G^*_{(km)} - G^{(1)}\right) + q\delta\left(G^*_{(km)} - G^{(2)}\right) + r\delta\left(G^*_{(km)} - G^{(3)}\right), \tag{2}$$

where $\delta\,(x)$ is a Dirac delta function. In Eq. (2) every bond is bounded with the closest neighbor nodes (km) in the lattices of N inner and N_Γ contact boundary nodes. It can either belong to component (1), (2) or (3) characterized by physical parameters $G^{(1)}$, $G^{(2)}$ and $G^{(3)}$ correspondingly.

We model global (or effective) properties of a material with randomly distributed local properties according to a real space renormalization group method introduced by Reynolds et al. [22–24]. The iterative transformation of generalized probability density function of Eq. (2) is defined as [8]

$$\rho_{n+1}\left(G^*_{(k'm')}\right) = \int_E \prod_{\substack{k\in S\setminus S_\Gamma \\ m\in S}}^{k\neq m} \left(dG^*_{(km)}\rho_n\left(G^*_{(km)}\right)\right)\delta\left(G^*_{(k'm')} - \left\langle F\left(\left\{G^*_{(km),n}\right\}\right)\right\rangle\right), \tag{3}$$

where

$$E = \left\{E^{(1)} \cup E^{(2)} \cup E^{(3)}\right\}. \tag{4}$$

S is a surface covering N inner and N_Γ nodes on Γ boundary, and $S \setminus S_\Gamma$ is a surface where nodes N_Γ are excluded. $\left\langle F\left(\left\{G^*_{(km),n}\right\}\right)\right\rangle$ is the effective susceptibility function of a lattice, delineated via a basic element bounded by nodes (km), which was averaged over all configurations E in a way to preserve the invariant form of Eq. (2) for every nth scale of recursive building of hierarchical lattice. In Eq. (4) the set E is a unification, $\cup$, of connected, $E^{(1)}$ and $E^{(2)}$, and any (i.e. connected and disconnected), $E^{(3)}$, clusters. What can be noted is that the number of elements in a set E is equal $3^5 = 243$ for the renormalization unit self-dual cell presented in Fig. 1(a).