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On multi-scale percolation behaviour of the effective conductivity for the lattice model with interacting particles

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HIGHLIGHTS

- We study the multi-scale site percolation in a system with interacting particles.
- At every scale, the interactions have a significant impact on the value of the critical concentration.
- When a repulsive interaction dominates the thermal energy, the exact critical concentrations at two small scales are found.
- At large scales, the highest possible value of the estimated threshold is given.

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ABSTRACT

Recently, the effective medium approach (EMA) using 2×2 basic cluster of model lattice sites to predict the conductivity of interacting microemulsion droplets has been presented by Hattori et al. To make a step aside from pure applications, we studied earlier a multi-scale percolation, employing any $k \times k$ basic cluster for non-interacting particles. Here, with interactions included, we examine in what way they alter the percolation threshold for any cluster case. We found that at a fixed length scale k, the interaction reduces the range of shifts of the percolation threshold. To determine the critical concentrations, the simplified EMA-model is used. It diminishes the number of local conductivities into two main ones. In the presence of a dominance of the repulsive interaction over the thermal energy, the exact percolation thresholds at two small scales can be revealed from analytical formulas. Furthermore, at large scales, the highest possible value of the estimated threshold can be obtained.

1. Introduction

One of the simple techniques to investigate essential physical properties of random heterogeneous materials is the network extension of effective medium approximation (EMA). A few years ago, Hattori et al. presented a lattice EMA-model that describes electrical percolation in the microemulsion solution with interacting droplets [1]. This is an important point because in a system of interacting particles, the percolation behaviour is influenced not only by the volume concentration, but also by the interactions between particles, which involve correlation of positions. As it was mentioned in Ref. [1], some microemulsion systems show both an electrical percolation phenomenon, whose concentration threshold depends strongly on temperature, and a phase separation. Thus, an analytical prediction of the relationship between the percolation threshold

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and interactions is of some importance. For these purposes, they make use of the basic cluster composed of only four unit cells. Despite this simplification, their results are in a qualitative agreement with the experimental data.

Instead of the 2×2 basic EMA-cluster of lattice sites used in Ref. [1], the earlier modification of this model takes into account any cluster's size $k \times k$, yet for zero interaction energy [2]. Such an approach can be treated as a high-temperature description of the initial lattice model. It was found that the location of the percolation threshold is k-dependent. In particular, an increase alone in the basic cluster's size modifies considerably the critical concentration, shifting it close to one.

In the multi-scale approach to the lattice EMA-model with interaction energy Δ between two adjacent conducting particles, which is proposed here, also the related chemical potential μ is accounted for. Here, we examine in what way the interactions alter the percolation threshold for any cluster case. We consider the physically sound range of interaction energies. On the one hand, the attractive interaction with $0 < \beta\Delta \leq 1$ is taken into consideration, where the standard notation $\beta \equiv 1/k_BT$ is applied, where k_B is the Boltzmann's constant and T denotes the temperature. On the other hand, the more important repulsive case with $-\infty < \beta\Delta < 0$ is also examined.

It is worth remarking that the interacting particles are treated as *non-overlapping* finite-size objects, that is, as unit square cells centred on the lattice sites [1]. Frequently, to consider effective properties/microstructure relations, computer simulations make use of digitized images of real samples [3–5]. However, we should bear in mind that the effective conductivity and percolation itself could be influenced by the size of mono-grains [6], as well as by the grain size distribution in a random material [7] or polydispersity [8]. The usage of the finite size objects can also be extended to percolation of dimers on square lattices [9] and further, to the impact of defects on percolation in random sequential adsorption of linear k-mers on square lattices [10]. Along this line, but for a three-dimensional (3D) system of straight rigid rods of length k, the ratio between percolation threshold and jamming coverage (θ_p/θ_j) shows a non-universal behaviour, monotonically decreasing to zero, with increasing k [11]. In turn, for a system consisting of overlapping squares or cubes, the percolation behaviour of obstacles and of the void space was carefully analysed, as well as the transition between continuous and discrete percolation [12]. This shortened list of papers making use of finite-size objects in the context of percolation phenomenon ends with the work devoted to 3D electric conductivity of overlapped spheroids of revolution in continuum [13]. The conductivity curves depend upon the shape of conductive spheroids while the percolation threshold shows a non-monotonic dependence on the related aspect ratio.

Here, we concentrate on two queries: (i) in what way at *fixed* scales the strength of the interactions modifies the system's percolation threshold and reversely, (ii) how a given interaction energy of adjacent particles influences the percolation behaviour at *different* length scales k. In that way, the work completes the earlier paper [2].

2. The model Z4 and its simplified version Z4s

Let us consider a scale extension of the two-dimensional regular lattice EMA-based model with M sites used by Hattori et al. [1]. Each of the sites can be occupied by a particle ($s_i = 1$), here represented by a unit lattice-distance, square cells 1×1, of the higher conductivity H-phase with the global volume concentration ϕ and a given electrical conductivity $\sigma_H \gg \sigma_L$. For the L-phase with the global volume concentration $\theta \equiv 1 - \phi$, its σ_L-conductivity is attributed to an empty cell ($s_i = 0$). We consider a general case of an elementary $k \times k$ cluster in the presence of interactions. Following the paper [1], we suppose that Hamiltonian of the system has the form:

$$\mathscr{H} = -\Delta \sum_{\langle ij \rangle} s_i s_j - \mu \sum_{i=1}^{M} s_i. \tag{2.1}$$

Here Δ is the interaction energy between two adjacent particles, μ is the chemical potential of the particle and summation on $\langle ij \rangle$ is over the nearest neighbour sites.

Inspired by the assumption used in Ref. [1], about neglecting fluctuations of electrical potential in the orthogonal direction to the macroscopic electric field directed along x-axis, we focus on investigation of a possible multi-scale behaviour of electrical percolation in such a model. At this stage, our main task is to obtain, at any fixed length scale k, the probability of appearance of a class of configurations $C_i(k)$, each of the local conductivity $\sigma_{x,i}(k) \equiv \sigma_i$ computed according to the formula

$$\sigma_i = \sum_{j=0}^{k} \frac{r_j}{j/\sigma_H + (k-j)/\sigma_L}. \tag{2.2}$$

Here, k denotes the number of rows, while the quantity $r_j \in \{r_0, \ldots, r_j, \ldots, r_k\}$ describes the number of rows with exactly j particles. It should be noticed that the local conductivity given by Eq. (2.2) is independent of the locations of particles in any row and of the permutations of rows, either, while the cluster energies are dependent on them.

We remind that the following obvious conditions should also be satisfied:

$$r_0 + r_1 + \cdots + r_k = k \tag{2.3a}$$

and

$$r_1 + 2r_2 + \cdots + k\, r_k = n_i, \tag{2.3b}$$