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Potts-model formulation of continuum percolation

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We present a continuum version of the Potts model, which can be used to describe both random and correlated continuum percolation.

The Potts-model formulations of both the random[1] and correlated[2–4] percolation models have been instrumental in our obtaining a deeper understanding of the percolation problem. They have also been essential to our understanding of the fundamental relation between thermal phase transitions and percolation.[3–6] These advances have all taken place in the context of lattice models. No parallel program has been devised for the problem of continuum percolation which would deepen our understanding of phase transitions in gel systems as well as fluids.

In this Brief Report we propose a Potts-like model, the continuum Potts model (CPM), which provides a Hamiltonian capable of describing both the random and correlated continuum percolation problems. We will present the model in the context of random percolation and then indicate the generalization to the correlated case.

The continuum random percolation problem is defined as follows: Consider a system containing N noninteracting d-dimensional spheres of diameter R in a volume V. Two spheres are said to be connected (i.e., belong to the same cluster) if they overlap; that is if the distance between spheres $x_{ij} < R$. A set of s spheres is said to be connected if any sphere selected at random from the set can be connected to any other sphere in the set by a path that only passes through overlapping spheres. Such a set is called an s particle cluster. This model has been studied with renormalization-group[7] and numerical methods[8] and is seen to undergo a percolation transition at a critical value of $\rho = N/V$ in the thermodynamic limit. The function that plays the role of the free energy in the percolation problem is the mean number of clusters[1] $\langle N_c \rangle$. Once this function is obtained all quantities of interest in the percolation problem can be calculated.

Consider then a system with the following Hamiltonian

$$-\beta H = \sum_{ij} v(x_{ij})(\delta_{\sigma_i \sigma_j} - 1) \ . \tag{1}$$

$\beta = 1/k_B T$, $\delta_{\sigma_i \sigma_j}$ is the Kronecker delta and $v(x_{ij}) = 0$ if $x_{ij} > R$ and $v(x_{ij}) = \infty$ if $x_{ij} \leq R$. The function $v(x_{ij})$ is simply the hard-sphere interaction. The sum $\sum_{ij}$ is over all pairs of particles. The term $(\delta_{\sigma_i \sigma_j} - 1)$ in Eq. (1) has the following interpretation. The particles can be thought of as having q internal states. If two molecules are in the same internal state then from Eq. (1) there is no interaction, however, if they are in different internal states there is a hard-core repulsion.

The main result of this Brief Report is that the mean number of clusters is obtained from Eq. (1) as follows

$$\langle N_c \rangle = \lim_{q \to 1} \frac{\partial}{\partial q} \ln z \ , \tag{2}$$

where

$$z = \sum_{\substack{\text{config} \\ \{\sigma\}}} \int \cdots \int \prod_i d\vec{x}_i \exp\left[\sum_{ij} v(x_{ij})(\delta_{\sigma_i \sigma_j} - 1)\right] \ . \tag{3}$$

This result can be obtained with the use of techniques similar to those developed in Ref. 1. We write

$$\exp\left[\sum_{ij} v(x_{ij})(\delta_{\sigma_i \sigma_j} - 1)\right] = \prod_{i<j} [(1 - e^{-v(x_{ij})})\delta_{\sigma_i \sigma_j} + e^{-v(x_{ij})}] \ . \tag{4}$$

Since $\lim_{q \to 1} z = V^N$, Eq. (2) becomes

$$\langle N_c \rangle = V^{-N} \lim_{q \to 1} \frac{\partial}{\partial q} \sum_{\substack{\text{config} \\ \{\sigma\}}} \int \cdots \int \prod_i d\vec{x}_i \prod_{c<j} [(1 - e^{-v(x_{ij})})\delta_{\sigma_i \sigma_j} + e^{-v(x_{ij})}] \ . \tag{5}$$

Consider the term in the expansion of the product in Eq. (5) of the form $\prod_{i<j} e^{-v(x_{ij})}$ which gives a contribution

to $\langle N_c\rangle$ of

$$V^{-N}\lim_{q\to 1}\frac{\partial}{\partial q}q^N\int\cdots\int\prod_i d\vec{x}_i\prod_{i<j}e^{-v(x_{ij})}=\frac{N}{V^N}\int\cdots\int\prod_i d\vec{x}_i\prod_{i<j}e^{-v(x_{ij})}\ . \tag{6}$$

In Eq. (6) the term

$$\int\cdots\int\prod_i d\vec{x}_i\prod_{i<j}e^{-v(x_{ij})}$$

is the phase-space volume occupied by the system of N particles with the condition that no particles overlap, and V^N is the total volume in phase space. The ratio of these two quantities is the probability that none of the N particles overlap. The right-hand side of Eq. (6) then is the mean number of one-particle clusters. Consider next the term in the expanded product of Eq. (5)

$$(1-e^{-v(x_{ij})})\delta_{\sigma_1\sigma_2}\prod_{\substack{i<j\\ i,j\neq 1,2}}e^{-v(x_{ij})}\ . \tag{7}$$

The corresponding contribution to $\langle N_c\rangle$ is then

$$(N-1)\int\cdots\int\prod_i d\vec{x}_i(1-e^{-v(x_{ij})})\prod_{\substack{i<j\\ i,j\neq 1,2}}e^{-v(x_{ij})}\ , \tag{8}$$

where the integral is the total phase-space volume occupied by the N particles with the constraint that particles 1 and 2 overlap and all others do not. Dividing the integral by V^N gives the probability of this configuration. If we took the sum of all terms constructed in this way with different pairs replacing 1 and 2, we would have the mean number of clusters in the case where one pair selected at random overlaps and all others do not. Clearly a continuation of this process will result in Eq. (2).

We point out here without going into details[1,9] that if we modify our Hamiltonian as follows,

$$-\beta H=\sum_{ij}v(x_{ij})(\delta_{\sigma_i\sigma_j}-1)+h\sum_i(\delta_{\sigma_i1}-1)\ , \tag{9}$$

then Eq. (2) is still valid with z constructed with the Hamiltonian of Eq. (9). The order parameter and mean cluster size are now related to the first and second derivatives of $\langle N_c\rangle$ with respect to h in the standard way.[1,9] It is interesting to note that the additional factor generated in the Boltzman factor by the $h(\delta_{\sigma_i1}-1)$ term in Eq. (9) $\{\exp[h(\delta_{\sigma_i1}-1)]\}$ can be thought of as a fugacity. The CPM can then be understood as describing a fluid (with a fixed number of particles N) with the Hamiltonian given in Eq. (1), however, the total number of particles with an internal state $\sigma_i\neq 1$ is not fixed but is governed by a fugacity e^{-h}.

It is also clear that we can generalize our system by adding to Eq. (9) an additional term $H_{\rm FL}$ which can be, for example, a Lennard-Jones potential or a square well, or any of the potentials useful in fluid theory. We have then

$$-\beta H=\sum_{ij}v(x_{ij})(\delta_{\sigma_i\sigma_j}-1)+h\sum_i(\delta_{\sigma_i1}-1)+H_{\rm FL}\ . \tag{10}$$

This Hamiltonian, in a way similar to that discussed above, describes correlated continuum percolation where the correlation is dictated by $H_{\rm FL}$.[10] The case $H_{\rm FL}$ consisting of only a hard-core interaction has been studied[11] via Monte Carlo renormalization group. A Mayer cluster approach to continuum percolation has also been proposed.[12]

In conclusion, we have proposed a continuum Potts model that is capable of describing both random and correlated continuum percolation. This model raises various questions. Among the more interesting is whether there exists a relation between the percolation transition in this model [with the Hamiltonian given by Eq. (10)] and the critical point of the fluid system specified by $H_{\rm FL}$. Such relations between percolation and thermal transitions have been found previously for lattice models.[3,4] Questions involving such a relationship as well as those involving the relation between the continuum percolation model and gelation are currently being investigated.

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