Number of bonds in the site-diluted lattices: sampling and fluctuations

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We have calculated analytically the mean value and the variance of the number of bonds on the lattices of dimension \(d\) for the given occupation of sites. We consider both kinds of site occupation: with the fixed concentration \(n_s\) of occupied sites and with the probability \(p\) for a site to be occupied. We found that the variance are smaller in the former case and not depends from the dimensionality of the hypercubic lattice. Whereas in the last case it grows with the space dimensionality. The ratio of variances are quite different in the limit of \(p \to 1\). Finally, we demonstrate the relevance of the level of fluctuations on the precision of energy calculations for the Ising model in the Monte Carlo simulations.

I. INTRODUCTION

There are two ways to generate on the lattice a sample with the randomly occupied sites [1]. The first one, with the fixed number \(s\) of occupied sites. This is the sampling from a ‘canonical ensemble’ for which in this paper we will use the name \(s\)-sampling. The second way, with a fixed probability \(p\) for a given site to be occupied, i.e. sampling from a ‘grand canonical ensemble’, or \(p\)-sampling. It is known that both methods lead in the 'thermodynamic' limit of infinite lattice size to the same results for the free energy per Ising spin being placed onto occupied sites of the lattice [2].

If one choose the probability \(p\) for the site to be occupied the concentration of bonds between the occupied sites on the infinite lattice are \(n_{SS} = p^2\). We named this bonds as \(SS\)-bonds. Similarly, the concentration of bonds between non-occupied sites (\(NN\)-bonds) is \(n_{NN} = (1 - p)^2\) and the concentration of bonds between occupied and non-occupied sites (\(SN\)-bonds) are \(n_{SN} = 2p(1 - p)\). Clearly, the sum of the three concentrations \(n_{SS} + n_{NN} + n_{SN}\) is the probability that each bond belongs to one of the three types and equal to unity.

In this paper we asking the following questions: i) how fluctuates the concentration of bonds on the hypercubic lattices depending on the concentration of occupied sites? ii) how this fluctuations depend on the way of sampling? iii) how this fluctuations depend on the lattice size?

We found analytically the answers on the all of the stated questions.

We start our analyses with the simple case of one-dimensional periodic lattice in Section [3]. In Section [3] we calculated the mean value and the variance of the number of bonds for the square lattice using the results of Section [3]. In the following Section [4] we generalize our results for the \(d\)-dimensional hypercubic lattice. We conclude our paper with the discussion of results in Section [4].

II. ONE-DIMENSIONAL LATTICE

A. \(s\)-sampling

Let us consider an one-dimensional lattice with \(L\) sites and periodic boundary (i.e. ring).

We are interested in the probability \(P(b; s, L)\) to have \(b\) bonds between \(s\) occupied sites. The number of occupied sites \(s\), the number of bonds between occupied sites \(b\) and the number of clusters of occupied sites \(k\) are connected by relation

\[
k = s - b.
\]

Then, the probability could be easily written as

\[
P(b; s, L) = \frac{L C_{s-1}^{k-1} C_{L-s-1}^{k-1}}{k C_L^s},
\]
where combinatorial coefficients \( C^{k-1}_{L-s-1} \) is the number of dispositions of \( s \) sites among the \( k \) clusters, \( C^{k}_{L-s} \) - the same for \( L-s \) empty sites, \( C^{k}_{L} \) - number of configurations with the \( s \) occupied sites from \( L \) possibilities, and, finally, \( L/k \) - the number of positions of \( k \) clusters on \( L \) sites. The probability are normalized

\[
\sum_{b=0}^{s-1} P(b; s, L) = \sum_{b=0}^{s-1} \frac{L C^{s-b}_{s-1} C^{s-b-1}_{L-s-1}}{(s-b) C^{s}_{L}} = 1. \tag{3}
\]

Now, the mean value of bonds \( \langle b \rangle \) are

\[
\langle b \rangle = \sum_{b=0}^{s-1} b P(b; s, L) = \frac{s(s-1)}{L-1} \tag{4}
\]

and the mean density of bonds are given by \( L >> 1 \)

\[
n_b = \langle b \rangle / L \approx n_s^2 - n_s(1 - n_s)/L, \tag{5}
\]

where \( n_s = s/L \) is the density of occupied sites.

The variation of the number of bonds \( \Delta b = \langle b^2 \rangle - \langle b \rangle^2 \) could be calculated in the same manner

\[
\Delta b = \sum_{b=0}^{s-1} b^2 P(b; s, L) - \left( \sum_{b=0}^{s-1} b P(b; s, L) \right)^2 = \frac{s(s-1)(L-s)(L-s-1)}{(L-1)^2(L-2)} \approx \frac{s^2(L-s)^2}{L^3} \tag{6}
\]

and the variance of the density of bonds \( \Delta n_b \) are equal to

\[
\Delta n_b \approx n_s^2(1 - n_s)^2 - n_s(1 - n_s)(4n_s^2 - 4n_s + 1)/L \tag{7}
\]

for \( L >> 1 \).

**B. p-sampling**

The probability distributions of the some quantity \( A \) in the case of s-sampling \( P(A; s) \) and those of the case of p-sampling \( P(A; p) \) are connected by

\[
P(A; p) = \sum_{s=0}^{L} P(A; s)C^{s}_{L}p^s(1-p)^{L-s}, \tag{8}
\]

therefore the probability to obtain exactly \( b \) bonds between two sites occupied with the (independent) probability \( p \) on the lattice of size \( L \) are

\[
P(b; p, L) = \sum_{s=0}^{L} \left( C^{s}_{L}p^s(1-p)^{L-s} \frac{L C^{k}_{s-1} C^{k-1}_{L-s-1}}{k C^{s}_{L}} \right) \tag{9}
\]

with \( k \) given by eq. \( \text{[8]} \) and the mean value of the bonds \( \langle b' \rangle \) in the case of p-sampling will be given by

\[
\langle b' \rangle = \sum_{b=0}^{s-1} b P(b; p, L) \equiv \sum_{s=0}^{L} \left( C^{s}_{L}p^s(1-p)^{L-s} \langle b \rangle \right) = Lp^2, \tag{10}
\]

(\text{where prime sign ' denotes the p-sampling averages}) and the corresponding variation \( \Delta b' \) are given by

\[
\Delta b' = \sum_{s=0}^{L} \left( C^{s}_{L}p^s(1-p)^{L-s} \left( \langle b \langle b \rangle \rangle - \langle b \rangle^2 \right) = Lp^2(1-p)(1 + 3p) \tag{11}
\]

for \( L \geq 4 \).

We have to stress here, that the mean density of the number of bonds \( n_p = p^2 \) and their variance \( \Delta n_p = p^2(1 - p)(1 + 3p) \) do not contain any finite size dependences in contrast with the case of s-sampling behaviour in \( \text{[3]} \) and \( \text{[8]} \).
III. SQUARE LATTICE

Let us calculate the mean value of the number of bonds and it’s variation for the square lattice with periodic boundary conditions.

A. p-sampling

On the square lattice with periodic boundaries, there are $L^2$ vertical and $L^2$ horizontal bonds. The number of bonds in each of $L$ columns and each of $L$ rows are the random variables. Their mean values $\langle b\rangle_i'$ are given by (10) and their variances by (11). Thus, the mean value of the number of bonds on 2d lattice are

$$\langle b\rangle_d'=2L^2p^2.$$  \(12\)

and their variance are given by \[3\]

$$\Delta b_d'=2L^2\sum_{i=1}^{2L} \Delta b_i' + 2L^2 \sum_{i,j} \text{Cov} \left( \langle b\rangle_i', \langle b\rangle_j' \right)$$  \(13\)

where $i < j$.

It is clear that the column-column (row-row) covariances are equal to zero, and the column-row covariances are the same for all columns and rows, and

$$\Delta b_d'=2L^2p^2(1-p)(1+3p) + 2L^2\text{Cov} \left( \langle b\rangle_{\text{column}}', \langle b\rangle_{\text{row}}' \right).$$  \(14\)

We have to compute now the column-row covariance $\text{Cov} \left( \langle b\rangle_{\text{column}}', \langle b\rangle_{\text{row}}' \right)$

$$\text{Cov} \left( \langle b\rangle_{\text{column}}', \langle b\rangle_{\text{row}}' \right) = \langle \langle b\rangle_{\text{column}}' \langle b\rangle_{\text{row}}' \rangle - \langle b\rangle'^2.$$  \(15\)

The first average are splitted into two parts. The first one, corresponds to all cases of distribution of occupied sites on columns and rows with the constraint that the intersection of row and column $x^{*}$ are occupied. The second one, corresponds to the states with the unoccupied intersection site.

$$\langle \langle b\rangle_{\text{column}}' \langle b\rangle_{\text{row}}' \rangle = p \langle \langle b|x^* = \text{occupied}\rangle^2 + (1-p) \langle \langle b|x^* = \text{unoccupied}\rangle^2$$  \(16\)

We omit here the algebra leading to the final expression for the variation of the number of sites on the two-dimensional lattice with the given probability $p$ for the site to be occupied

$$\Delta b_d'=2L^2p^2(1-p)(1+7p).$$  \(17\)

Details will be published elsewhere \[4\].

B. s-sampling

We calculate also the mean value of the number of bonds on the square lattice with the linear size $L$ and with the fixed number $s$ of occupied sites

$$\langle b\rangle_d=\frac{2s(s-1)}{L^2-1}.$$  \(18\)

and the variance are

$$\Delta b_d=\frac{s(s-1)(L^2-s)(L^2-s-1)(2L^2-10)}{(L^2-1)^2(L^2-2)(L^2-3)}.$$  \(19\)
IV. HYPERCUBIC LATTICES

The mean value of the number of bonds on the $d$-dimensional hypercubic lattice with the probability $p$ for the site to be occupied are

$$\langle b \rangle_d = dL^d p^2.$$  \hfill (20)

The variance could be calculated in the same manner as in the two dimensional $d = 2$ case described above in the Section II A

$$\Delta b_d = dL^d p^2(1 - p) (1 + (4d - 1)p).$$ \hfill (21)

The explicit mean value and the variance of the number of bonds for the case of the fixed number $s$ of occupied sites could be calculated using (20) and (21) with the proposition that the mean value are quadratic in $s$. The result are

$$\langle b \rangle_d = \frac{ds(s - 1)}{L^d - 1}$$ \hfill (22)

and

$$\Delta b_d = \frac{ds(s - 1)(L^d - s)(L^d - s - 1)(L^d - 2d - 1)}{(L^d - 1)^2(L^d - 2)(L^d - 3)}$$ \hfill (23)

for $L > 2$.

The expressions we checked by direct enumeration in $d = 2$ for $L = 4, 5$ and in $d = 3$ for $L = 3$.

V. DISCUSSION

We do not find any evidence for the absence of self-averaging in the number of bonds. In the case of p-sampling the normalized variance

$$R_{b_d} = \frac{\Delta b_d}{\langle b \rangle_d^2} = \frac{1 - p}{p^2L^d} \propto L^{-d}$$ \hfill (24)

inverse proportional to the lattice volume. Therefore the number of bonds are the strong averaging quantity.

The normalized variance in the case of s-sampling

$$R_{b_d} = \frac{\Delta b_d}{\langle b \rangle_d^2} = \propto \frac{(1 - n_s)^2}{dL^{-d}n_s(n_s - 1/L^d)}$$ \hfill (25)

are nonmonotonic in $L$ and the strong self-averaging take place for $L > (1/n_s)^{1/d}$.

The relative variance for two cases

$$\frac{\Delta b_d}{\Delta b_d} = \frac{p^2(1 + (4d - 1)p)(1 - p)}{(n_s(1 - n_s))^2}$$ \hfill (26)

shows that in the limit of $p \to 1$ and $n_s \to 1$ the ratio diverges.

It is possible to give the physical interpretation to the last expression. Let us place Ising spin at each occupied site. Then, the energy $E_0$ at zero temperature will be equal to the number of bonds between the sites occupied by spins. The magnetization $M_0$ are equal to the number of occupied sites. Then, the ratio (26) are equal to the ratio $N_p/N_s$ of the number of samples ($N_p$ for the p-sampling and $N_s$ for the s-sampling) over which we have to average energy $E_0$ in order to get the same dispersion $\sigma E_0 = \sqrt{\Delta b/(N_x - 1)}$ of the energy $E_0$, where $N_x$ are either $N_p$ or $N_s$.

Finally, we could propose the third way to generate the samples, sb-sampling: get random samples with the fixed number of sites $s$ and choose among them only those which contain the "right" number of bonds $b = ds^2$. The results of Monte Carlo simulations for site diluted Ising model on square lattice had show that the dispersions of thermodynamic quantities like energy, specific heat and magnetic susceptibility are quite smaller for the proposed sb-sampling in comparison with both, s-sampling and p-sampling at all temperatures.
VI. ACKNOWLEDGMENTS

Authors are thankful to K. Binder for the kind discussion and suggestion to write this manuscript. The work is partially supported by grants from RFBR (99-02-18412), NWO and INTAS. O.A.V. is grateful to Landau stipendium committee (Forschungszentrum/KFA, Jülich) for support.

[1] L.N. Shchur, Incipient Spanning Clusters in Square and Cubic Percolation, in Springer Proceedings in Physics, "Computer Simulation Studies in Condensed Matter Physics XII", Eds. D.P. Landau, S.P. Lewis, and H.B. Schüttler, (Springer-Verlag, Berlin, 2000)
[2] R.B. Griffiths and J.L. Lebowitz, J. Math. Phys. 9 (1968) 1284
[3] W. Feller, An introduction to probability theory and its applications (John Wiley & Sons, New York, 1970)
[4] O.A. Vasilyev, to be published.
[5] B. Derrida and H. Hilhorst, J. Phys. C: Solid State Phys. 14 (1981) L539
[6] K. Binder, D.W. Heermann, Monte Carlo Simulations in Statistical Physics (Springer-Verlag, Berlin, 1997)
[7] S. Wiseman and E. Domany, Phys. Rev. E 52 (1995) 3469; Phys. Rev. Lett. 81 (1998) 22; Phys. Rev. E 58 (1998) 2938
[8] A. Aharony and A. B. Harris, Phys. Rev. Lett. 77 (1996) 3700; A. Aharony, A. B. Harris and S. Wiseman, Phys. Rev. Lett. 81 (1998) 252