Scaling law of Wolff cluster surface energy

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March 22, 2022

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Abstract

We study the scaling properties of the clusters grown by the Wolff algorithm on seven different Sierpinski-type fractals of Hausdorff dimension $1 < d_f \leq 3$ in the framework of the Ising model. The mean absolute value of the surface energy of Wolff cluster follows a power law with respect to the lattice size. Moreover, we investigate the probability density distribution of the surface energy of Wolff cluster and are able to establish a new scaling relation. It enables us to introduce a new exponent associated to the surface energy of Wolff cluster. Finally, this new exponent is linked to a dynamical exponent via an inequality.

Keyword: Wolff algorithm, fractal, surface energy, dynamical exponent, scaling law.

PACS:
64.60.Ak Renormalization-group, fractal, and percolation studies of phase transitions
68.35.Md Surface thermodynamics, surface energies
75.40.Mg Numerical simulation studies
89.75.Da Systems obeying scaling laws
In 1966, Kadanoff proposed an intuitive renormalization picture [1] to explain the Widom’s phenomenological hypothesis [2]. This hypothesis states a homogeneous transformation of the singular part of the free energy per spin under a change of length unit from 1 to $b$ in the vicinity of the critical temperature $T_c$ and can be written as

$$f(t, h) = b^{-d} f(b^{y_t} t, b^{y_h} h),$$

where $d$ is the integer space dimension of a translationally invariant system; the reduced temperature $t = T/T_c - 1$ and the external field $h$ are supposed to be small; $y_t$ and $y_h$ are two exponents associated with the two relevant directions of the renormalization flows. One notices that a translationally invariant system of dimension $d$ is auto-similar and can be considered as a particular case of fractal. In the case of a general fractal system, the translational symmetry is broken; however, a generalization of the space dimension can be done by introducing the Hausdorff dimension $d_f$. The number of spins on such system can be written as $N = L^{d_f}$ where $L$ is the network size. Thus, the Widom’s hypothesis can be generalized by replacing the factor $b^{-d}$ in Eq. (1) by $b^{-d_f}$ to describe the decrease of the effective number of spins during the change of the length scale. Since fractals are constructed by iteration of a generating cell, $b$ cannot take any value; it must be chosen so that the fractal structure remains invariant under the change of length unit. The critical behaviors of spin models on fractals whose Hausdorff dimension lies between 1 and 3 have been studied intensively by Monceau and Hsiao and co-workers [3, 4, 5, 6] and Carmona et al. [7], by performing Monte Carlo simulations. The results show the validity of the above generalization. More recently, a direct verification of the Kadanoff’s real space renormalization group picture of the Ising model in the case of a Sierpinski fractal has been achieved by Hsiao and Monceau [8]; they used a Monte Carlo renormalization group method.

The simulation works mentioned above have been mainly performed with the help of the Monte Carlo Wolff algorithm [9]. This algorithm is able to reduce efficiently the critical slowing down. Instead of involving a single-spin flip at each update of the spin state configuration, the Wolff algorithm grows firstly a cluster (so-called Wolff cluster) and then updates the state configuration by assigning a new state to the spins of this
Much information on the critical behavior of a discrete spin system can be brought out from the geometrical properties of the Wolff clusters. It has been shown that the mean size of Wolff clusters for the Ising model scales as $L^{\gamma/\nu}$ at $T_c$ where $\gamma$ and $\nu$ are the critical exponents associated to the susceptibility and the correlation length \[9\]. It provides an alternative way to calculate $\gamma/\nu$. Monceau and Hsiao checked that the values of $\gamma/\nu$ calculated from the Wolff mean cluster sizes are consistent with the ones calculated from the behavior of the maxima of the susceptibility with respect to $L$ in the case of the Sierpinski fractals with Hausdorff dimensions between 1 and 3.\[10\] \[11\] Moreover, the most striking result they carried out is the scaling invariance of the Wolff cluster size probability densities $\mathcal{P}(s)$ under a suitable rescaling. This scaling law holds at the critical point and reads

$$\mathcal{P}(s) = b^{-d_f} \mathcal{P}(b^{-x}s),$$

(2)

where $s$ denotes the size of Wolff cluster associated with a Monte Carlo step and $b$ is some appropriate change of length scale which keeps invariant the fractal structure. They proved that the exponent $x$ is equal to $y_h = \beta/\nu + \gamma/\nu$ where $\beta$ is the critical exponent associated to the magnetic moment. This scaling law can be understood as a decrease of Wolff cluster size by a factor $b^{y_h}$ under the change of the length scale $1 \rightarrow b$. During the simulations of the Ising model, the total magnetization $M$ and the total energy $E$ are calculated at each update of the spin state configuration. As a matter of fact, the absolute difference $|\Delta M|$ between two successive values of $M$ is equal to two times the size of the Wolff cluster grown during a Monte Carlo step. Hence, the scaling law described in Eq. (2) is satisfied by the probability density distribution of $|\Delta M|$. It is worth noticing that the mean absolute difference $|\Delta E|$ between two successive values of the total energy represents two times the surface energy of the Wolff cluster. Thus, there is much to learn in studying the scaling properties of $|\Delta E|$ and the associated probability density distribution. The purpose of this paper is to study the behavior of the surface energy of Wolff clusters grown on fractal lattices at the critical point. We investigate seven different Sierpinski-type fractals of Hausdorff dimension lying between 1 and 3. The lattices are generated iteratively from some generating cells and denoted $SP(\ell^d, n_{occ}, k)$. 
\( \ell \) is the size of the generating cell, \( d \) is the integer space dimension in which the lattice is embedded, \( n_{\text{occ}} \) is the number of occupied sites in the generating cell, and \( k \) is the number of iteration steps. Ising spins are placed at each center of the occupied sites. The size of \( SP(\ell^d, n_{\text{occ}}, k) \) is \( L = \ell^k \) and the number of spins is \( N = n_{\text{occ}}^k \). The Hausdorff dimension is defined by \( d_f = \log N / \log L = \log n_{\text{occ}} / \log \ell \). The true mathematical fractal is obtained only when \( k \) tends to infinity; in this case, we denote it by \( SP(\ell^d, n_{\text{occ}}) \). The structure of the fractal is not indicated in these symbols. The seven generating cells \( SP(\ell^d, n_{\text{occ}}, 1) \) we have chosen are

1. \( SP(2^2, 4, 1) \): a 2 by 2 square,
2. \( SP(3^2, 8, 1) \): a 3 by 3 square where the center sub-square is removed,
3. \( SP(5^2, 24, 1) \): a 5 by 5 square where the center sub-square is removed,
4. \( SP(2^3, 8, 1) \): a cube of size 2,
5. \( SP(3^3, 26, 1) \): a cube of size 3 where the center sub-cube is removed,
6. \( SP(4^3, 56, 1) \): a cube of size 4 where the center sub-cubes of size 2 are removed,
7. \( SP(3^3, 18, 1) \): one removes in addition the 8 sub-cubes at the corners of \( SP(3^3, 26, 1) \).

\( SP(2^2, 4) \) and \( SP(2^3, 8) \) are exactly a square and a cubic lattice of infinite size. It has been shown that the Ising model exhibits a second order ferromagnetic phase transition on a fractal, provided that the lattice has a particular geometrical property: the ramification order must be infinite [12]. It is the case for the fractals studied here. Moreover, the critical temperatures \( T_c \) on these fractals are available [4, 5, 13, 14] and their values are recalled in the table 1. The mean absolute value of the Wolff cluster surface energy can be calculated from the relation

\[
\frac{1}{2} \langle |\Delta E| \rangle = \frac{1}{2(N_{\text{sim}} - 1)} \sum_{n=1}^{N_{\text{sim}} - 1} |E_{n+1} - E_n|
\]

where \( N_{\text{sim}} \) is the total number of Monte Carlo steps and \( E_n \) is the total energy of the \( n \)-th updated configuration. Firstly, we found that \( \langle |\Delta E| \rangle \) follows power laws at \( T_c \) with respect to the lattice size \( L \) in the case of the seven different fractals we investigated.
It enables to define a surface exponent: $\langle |\Delta E| \rangle \sim L^{S_W}$. Fig.1 shows the behavior of $\langle |\Delta E| \rangle$ as a function of $L$ in logarithmic coordinates. The points line up along straight lines except for the small sizes, where the scaling corrections due to the finite-size effects are expected. It has been suggested that these corrections have a topological character and are linked to the slow convergence towards the thermodynamical limit in the case of the fractals with broken translational symmetry [5]. As a matter of fact, $\langle |\Delta E| \rangle$ follows perfectly a power law in the case of the translationally invariant lattices $SP(2^2, 4, k)$ and $SP(2^3, 8, k)$ where $L$ increasing as a geometrical series covers many orders of magnitude. We report the measured surface exponent $S_W$ in the table 1, where least-square fits are performed from $k = 8$ to 12 for $SP(2^2, 4, k)$, from $k = 5$ to 8 for $SP(2^3, 8, k)$, from $k = 4$ to 8 for $SP(3^2, 8, k)$, from $k = 2$ to 4 for $SP(4^3, 56, k)$, from $k = 3$ to 5 for $SP(5^2, 24, k)$, for $SP(3^3, 18, k)$, and for $SP(3^3, 26, k)$, respectively. On the other hand, since Monte Carlo simulations can be performed only on lattices of finite size and we have omitted the small-size data when extrapolating the thermodynamical limit, a slow crossover behavior may be interpreted as an asymptotic one. A detailed study shows that the points in Fig.1 exhibit a very slight concavity. The reported value $S_W$, hence, should be taken as an upper bound in a strict sense; however, the real thermodynamical-limit value is expected to be very close to the reported one.

We are now able to go further and study the scaling properties of the probability density distributions $P(|\Delta E|)$ of Wolff cluster surface energy. The curves showing $P(|\Delta E|)$ are similar to each other in logarithmic coordinates. These results suggest to write down a homogeneous transformation under the form:

$$P(|\Delta E|) = b^{-D_S}P(b^{-y_S}|\Delta E|),$$

(4)

where $D_S$ and $y_S$ are some introduced exponents. An intuitive guess is to set $D_S$ equal to $d_f - 1$ since it describes the usual surface dimension of a system of bulk dimension $d_f$. According to Eq.(4), $\langle |\Delta E| \rangle$ should scale as:

$$\langle |\Delta E| \rangle = \int_0^\infty |\Delta E|P(|\Delta E|) d|\Delta E|$$

$$= \int_0^\infty |\Delta E|b^{-(d_f-1)}P(b^{-y_S}|\Delta E|) d|\Delta E|$$

$$= b^{-(d_f-1)+2y_S} \int_0^\infty |\Delta E'|P(|\Delta E'|) d|\Delta E'|,$$
where we have performed the change of variable $|\Delta E'| = b^{-y_S}|\Delta E|$. Since the correlation length is divergent at $T_c$, we can set $b$ equal to the lattice size $L = \ell^k$. $\langle |\Delta E| \rangle$ is, therefore, proportional to $L^{-(d_f-1)+2y_S}$. We are, hence, able to obtain a relation linking the exponents $S_W$ and $y_S$:

$$S_W = -(d_f - 1) + 2y_S.$$  \hspace{1cm} (5)

The values of $y_S$ calculated from Eq.(5) for the seven fractals investigated are given in the table 1.

The similarity property of the curves showing the probability density distributions $P(|\Delta E|)$ and the validity of the homogeneous transformation Eq.(4) can be brought out in the following way: for a given structure at different values of the iteration step $k$, the curves showing $P(|\Delta E|)$ collapse onto the one corresponding to the lattice of the largest size $L = \ell^{k_{max}}$ under the mapping:

$$ (|\Delta E|, P(|\Delta E|)) \rightarrow (\ell^{(k_{max}-k)y_S}|\Delta E|, \ell^{-(d_f-1)(k_{max}-k)}P(|\Delta E|)) .$$

Fig.2 shows such collapses for the three largest values of $k$ on the fractals $SP(3^2,8)$, $SP(2^2,4)$, and $SP(3^3,18)$. These data-collapses work out in a reliable way with the values of $y_S$ given in Table 1. It confirms that $D_S$ is equal to $d_f - 1$ (It has also been checked for the four other fractals). Furthermore, $P(|\Delta E|)$ does not exhibit a peak as $P(s)$ does. The effect of segregation between large and small clusters mentioned in Ref.[10, 11] is smoothed in the behavior of $P(|\Delta E|)$. It means that an important part of the simulation is carried out in updating large clusters; however, the update of the large clusters does not necessarily imply a large change of the total energy. For a given cluster size, the probability distribution of the border surface is broad.

A fundamental question is to know if the introduced exponent $y_S$ is a new one, that is, if it is independent of the two renormalization group eigen-exponents $y_t$, $y_h$ and the Hausdorff dimension $d_f$. To our knowledge, it’s the first time that the surface energy scaling property of Wolff cluster is investigated. No analytical or theoretical treatment is available. According to our Monte Carlo simulation results (table 1), $y_S$ seems to be independent of $y_t$, $y_h$ and $d_f$. Whether $y_S$ links to some of the surface exponents of a bulk system [15] remains an open question. In the table 1, regardless of the fractal structures,
one can find that the values of $y_t$, $y_h$ and $y_S$ increase as the Hausdorff dimension $d_f$ increases. Moreover, we do not expect that $\epsilon$-expansion results can be interpolated to non-integer dimensions and provide the values of $y_t$ and $y_h$ on the fractals, even the value of $y_S$. Accurate Monte Carlo studies have shown that the universality of phase transitions on the hierarchical lattices without translational symmetry should depend on the lattice structure \[4, 5\]. Hence, $y_S$ associated to the fractals with broken translational symmetry depends on the lattice structure too.

As the Wolff clusters are dynamical objects, we exploit here the connection between the surface exponent $y_S$ and the dynamical scaling exponent. We firstly study the mean square surface energy of Wolff cluster

$$\langle (\Delta E)^2 \rangle = \frac{1}{N_{sim}-1} \sum_{n=1}^{N_{sim}-1} (E_{n+1} - E_n)^2.$$ (6)

We find that $\langle (\Delta E)^2 \rangle$ lines up along straight lines with respect to $L$ except for the small lattice sizes in logarithmic coordinates for the seven fractals investigated (see Fig.3). The associated exponent $u$, defined by $\langle (\Delta E)^2 \rangle \sim L^{2u}$, could be measured in the same way as described in the previous text for the exponent $S_W$; the values of $u$ are reported in the table 1. We, then, express $\langle (\Delta E)^2 \rangle$ as $2 [\langle E^2 \rangle - \langle E \rangle^2] (1 - \theta_{EE}(1))$ where $\theta_{EE}(n) = (\langle E_0 E_n \rangle - \langle E \rangle^2) / (\langle E^2 \rangle - \langle E \rangle^2)$ is the normalized autocorrelation function. Since the autocorrelation time is much longer than 1 (in some appropriate time unit), $1 - \theta_{EE}(1)$ represents approximatively the negative derivative of the autocorrelation function at the origin. It enables to define a statistic-fluctuation autocorrelation time $\tau_{sf}^E$ and an associated dynamical exponent $z_{sf}^E$: $-(d\theta_{EE}(t)/dt|_{t=0}) = (\tau_{sf}^E)_{-1} \sim L^{-z_{sf}^E}$.\[16\] Notice that, according to Eq.(1), the term $\langle E^2 \rangle - \langle E \rangle^2$ should asymptotically scale as $L^{\alpha/\nu + d_f} = L^{2/\nu}$ at $T_c$, where $\alpha$ is the critical exponent associated to the specific heat per spin $c_v$. One should keep in mind that the non-singular part of the free energy per spin gives, in addition, an important contribution in determination of the critical behavior of $c_v$ \[4\]. We, therefore, have $2u = 2\nu^{-1} - z_{sf}^E$ in the thermodynamical limit. With the help of the inequality $|\langle \Delta E \rangle| \leq \sqrt{\langle (\Delta E)^2 \rangle}$, we can link the surface exponent $S_W$ with the dynamical one $z_{sf}^E$ in the following way: $S_W$ is upper bounded by $u = \nu^{-1} - z_{sf}^E/2$. Moreover, since $\langle (\Delta E)^2 \rangle$ follows a power law, a homogeneous transformation for the probability density
of \((\Delta E)^2\) can be stated; it takes the following form

\[
P((\Delta E)^2) = b^{-2(d_f-1)}P(b^{-y}(\Delta E)^2),
\]

and has been verified on the seven fractals investigated here. In this case, \((\Delta E)^2\) decreases by a factor \(b^y = b^{\alpha+(d_f-1)}\) under a suitable change of length unit \(1 \to b\). A similar process could be applied in the study of Wolff cluster size or the successive change of total magnetic moments. One can show that \(\langle |\Delta M| \rangle \leq \sqrt{\langle (\Delta M)^2 \rangle}\) and, therefore, \(\gamma/\nu\) is upper bounded by \((\gamma/\nu + d_f - z_{sf}^M)/2\) where \(z_{sf}^M\) is the statistic-fluctuation dynamical exponent associated to the total magnetic moment. It implies \(z_{sf}^M \leq d_f - \gamma/\nu = 2\beta/\nu\).

The method developed in this paper can be generalized to the study of some physical quantity whose mean value follows a power law with respect to \(L\). For instance, since \(\langle |M| \rangle \sim L^{y_h}\) at \(T_c\), one can verify, by constructing a homogeneous transformation for the probability density of \(|M|\) similar to Eq.(2), that \(|M|\) decreases by a factor \(b^{(y_h+d_f)/2}\) under a suitable rescaling \(1 \to b\). All these results suggest that the scaling properties of some physical quantity at \(T_c\), where the correlation length is divergent, comes originally from the underlying hierarchal structure of a fractal.

In summary, we have studied the scaling properties of the Wolff cluster surface energy in the framework of the Ising model in the case of seven different fractals dimensions. A new scaling relation for the absolute value of the surface energy \(|\Delta E|\) of the Wolff’s cluster has been established. We have shown that \(|\Delta E|\) scales as \(b^{-y_s}|\Delta E|\) under an increment of the length unit by the factor \(b\), which remains invariant the underlying structure of the fractal. Finally, the surface exponent \(S_W\) is proved to be upper bounded by \(\nu^{-1} - z_{sf}^E/2\).

Acknowledgements A part of the numerical simulations was carried out in the Institut de Développement et des Ressources en Informatique Scientifique, supported by the Centre National de la Recherche Scientifique (project No. 021186). We acknowledge the scientific committee and the staff of the center. We are also grateful to the Centre de Calcul Recherche of the University Paris VII—Denis Diderot, where the rest of the simulations have been performed.
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Table 1: Measured values of $S_W$ and $u$ on the seven fractals. $y_S$ is calculated from Eq.(5). The values of $T_c$, $y_t$ and $y_h$ are recalled from Ref.[8], Ref.[5], Ref.[14], Ref.[4], and Ref.[13].

| fractal  | $T_c$    | $y_t$   | $y_h$   | $S_W$    | $y_S$    | $u$     |
|----------|----------|---------|---------|----------|----------|---------|
| $SP(3^2,8)$ | 1.4795(5) | 0.449(6) | 1.8198(11) | 0.838(2) | 0.865(1) | 0.878(4) |
| $SP(5^2,24)$ | 2.0660(15) | 0.923(2) | 1.861(5) | 0.8188(2) | 0.8967(1) | 0.880(2) |
| $SP(2^2,4)$ | $2/\ln(1 + \sqrt{2})$ | 1 | 1.875 | 0.8100(2) | 0.9050(1) | 0.8777(8) |
| $SP(3^3,18)$ | 2.35090(9) | 1.185(16) | 2.317(16) | 0.849(8) | 1.240(4) | 1.016(9) |
| $SP(4^3,56)$ | 3.99893(10) | 1.410(36) | 2.407(14) | 0.742(10) | 1.323(5) | 0.990(11) |
| $SP(3^3,26)$ | 4.21701(6) | 1.503(53) | 2.449(22) | 0.738(2) | 1.352(1) | 0.995(5) |
| $SP(2^3,8)$ | 4.511516(41) | 1.588(2) | 2.482(2) | 0.759(5) | 1.3795(25) | 1.018(5) |
Figure captions

Fig.1 $\langle |\Delta E| \rangle$ versus lattice size $L$ on the seven fractals investigated in logarithmic coordinates.

Fig.2 Collapses of $\mathcal{P}(|\Delta E|)$ on the fractals $SP(3^2, 8, k)$, $SP(2^2, 4, k)$ and $SP(3^3, 18, k)$ under the mapping described in the text.

Fig.3 $\sqrt{\langle (\Delta E)^2 \rangle}$ versus lattice size $L$ on the seven fractals investigated in logarithmic coordinates.
\[ |\Delta E| \leq L \]

Graph showing the relationship between \(|\Delta E|\) and \(L\) for various Lie algebras. The graph includes data points for different Lie algebras labeled as:
- \(\text{SP}(2^2, 4,k)\)
- \(\text{SP}(3^2, 8,k)\)
- \(\text{SP}(2^3, 8,k)\)
- \(\text{SP}(3^3, 26,k)\)
- \(\text{SP}(4^3, 56,k)\)
- \(\text{SP}(3^3, 18,k)\)
- \(\text{SP}(2^2, 4,k)\)
- \(\text{SP}(5^2, 24,k)\)
- \(\text{SP}(3^2, 8,k)\)
$P(|\Delta E|) \rightarrow P'(|\Delta E'|)$

- $SP(3^2, 8, k)$
  - $k=6$
  - $k=7$
  - $k=8$

- $SP(2^2, 4, k)$
  - $k=10$
  - $k=11$
  - $k=12$

- $SP(3^3, 18, k)$
  - $k=3$
  - $k=4$
  - $k=5$
