Low–Temperature Series for Renormalized Operators: the Ferromagnetic Square–Lattice Ising Model

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Abstract

A method for computing low-temperature series for renormalized operators in the two-dimensional Ising model is proposed. Series for the renormalized magnetization and nearest-neighbor correlation function are given for the majority rule transformation on 2×2 blocks and random tie-breaker. These series are applied to the study at very low temperature of the first-order phase transition undergone by this model. We analyze how truncation in the renormalized Hamiltonian leads to spurious discontinuities of the Renormalization Group transformation.

Keywords: Renormalization group, position–space renormalization–group transformations, Ising model, low–temperature expansions.

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1 Introduction

The behavior of the Renormalization Group (RG) in the vicinity of first order phase transitions has been a very controversial matter for the last 20 years. In 1975 Nienhuis and Nauenberg [1] proposed that the RG transformations behave near first-order transition points in a similar fashion as near standard critical points. Each RG step is smooth (i.e. the renormalized couplings are analytic functions of the original ones, even at the transition points). Singular behavior is recoved as we infinitely iterate this transformation near a fixed point. Moreover, first-order transition points are governed by a so-called "discontinuity fixed point" (DFP), characterized by i) A domain of attraction which includes the transition surface. ii) Zero correlation length (In most systems, first-order transition points possess a finite correlation length. See [2] for a counterexample). iii) A relevant operator whose critical exponent is given by the dimensionality of the system y = d. As a matter of fact, there are as many exponents y = d as phases coexist at the transition line ¹ [3]. In the Ising model it is believed that the DFP is located at zero temperature [4].

This picture was criticized by some authors [5, 6, 7, 8, 9] who claimed that the RG flow is itself discontinuous at the transition line. That is, they claimed that the renormalized Hamiltonian has different limiting values depending on how the original Hamiltonian approaches the transition line. As a result, they doubted whether the DFP would exist at all. Most of these claims were based on Monte Carlo Renormalization Group (MCRG) computations. In ref. [9] non-rigorous analytical arguments were given to support the same conclusion. In ref. [10] it was argued that the observed discontinuities are artifacts due to the truncation of the Hamiltonian space inherent in the MCRG approach. In fact, for the two-dimensional Ising model and majority rule with 2×2 blocks it was found that the discontinuity in the magnetic field was of the same order as the truncation error. Moreover, as the number of operators included in the computation was increased, the size of this discontinuity decreased.

This puzzle was solved partially by van Enter-Fernández-Sokal [11], who showed that for systems with bounded dynamical variables and interacting through a Hamiltonian belonging to the space \mathcal{B}^1 (i.e. the space of real, absolutely summable and translation-invariant interactions) the RG flow is always continuous and single-valued, whenever it exists at all (subject to some very mild locality conditions on the RG transformation). For finite systems the existence of the transformation (i.e. of the renormalized Hamiltonian) is trivial. In the thermodynamic limit, however, this is a very subtle problem. As a matter of fact, these authors proved that the renormalized Hamiltonian does not exist in the two-dimensional Ising model when the temperature is low enough, for the Kadanoff transformation, decimation, block average and some particular cases of majority rule. On the other hand the majority rule with blocks of size b = 2 (the case most considered in the literature) is still an open problem. Notice that the pathologies always occur at low temperatures. In such a regime there is an alternative to MCRG computations: the low-temperature (low-T) expansions [12, 13, 14, 15, 16].

In this paper we propose to study the behavior of several RG transformations using low-T expansions. This approach has several advantages over MCRG computations. MCRG methods have three sources of errors: statistical errors, finite-size effects and truncation errors. Series expansions do not suffer from the first two, as the observable quantities are obtained directly in the thermodynamic limit and no stochastic process is involved². If we wished to obtain a renormalized Hamiltonian from the renormalized expectation values, then a truncation scheme would be involved. However, in this paper we will use our results to study the truncation procedure itself and learn why it works or does not work.

If we truncate the renormalized Hamiltonian (i.e. we allow only a finite number of renormalized interactions), we can obtain estimates for those couplings by solving a highly non-linear set of equations, which involve expectation values of operators computed in the renormalized measure. In this paper we develop a procedure to compute series expansions for these expectation values, which have not been computed previously (to our knowledge) in the literature. For real-space RG transformations the expectation value of an operator O with respect the renormalized measure can be written as an expectation value in the original measure of a certain composite operator \tilde{O} . This composite operator \tilde{O} is equal to the original operator O acted upon by a probability kernel (which is the mathematical object representing the RG transformation). Thus, if we know how to obtain the low-T expansions in the original

 $^{^{1}}$ Here we take into account the (trivial) critical exponent associated with the renormalization of the identity operator in the Hamiltonian.

²Note that unlike many applications of series expansions, here we are really interested in the behavior at low temperature and *not* in the critical region $T \approx T_c$. Therefore, no extrapolation procedure is involved.

(or unrenormalized) measure, then we can compute any expectation value by doing the corresponding integral.

These series can be useful in two other ways: i) They provide a real check for MCRG computations at low temperature. Expectation values coming from the Monte Carlo simulations can be compared with the low-T predictions. ii) When performing a RG transformation the system is viewed at a larger spatial scale. For that reason we believe that the low-T series for the renormalized magnetization, susceptibility and specific heat could be used to extract the critical exponents (using standard series-extrapolation techniques). In fact, a better convergence could be expected for these "improved" series. It would be interesting to devise a computational procedure to generate these series to an arbitrary order.

On the other hand, the main goal of this paper is to analyze the truncation issue in the Ising model. Starting at the first order transition line and at very low temperature, we would like to know whether it is possible to obtain estimates for the renormalized couplings in such a way that the truncated interaction does not contain any odd term. An affirmative answer would imply that the approximate RG transformation, restricted to some finite-dimensional subspace of \mathcal{B}^1 , is continuous at the transition line. We find that this situation occurs for the majority rule transformation (on 2×2 blocks) when restricted to a subspace containing a magnetic field and a nearest-neighbor interaction. On the other hand, we find that this is not the case for the decimation and large-p Kadanoff transformations restricted to the latter two-dimensional subspace or for the majority rule transformation when restricted to the three-dimensional subspace containing magnetic field, nearest-neighbor and next-to-nearest-neighbor interactions. In all of these cases, the renormalized magnetic field is *non-zero* implying that the approximate RG map is *discontinuous*. Thus, the typical situation seems to be that truncation induces discontinuities in the RG transformation when restricted to some finite-dimensional subspace of the interaction space. However, the relation between these results on truncation and the results of [11] on non-Gibbsianness is far from clear.

This paper is organized as follows. In Section 2 we describe the way the low-T expansions for renormalized observables can be obtained. We give three examples for the two-dimensional Ising case: decimation, Kadanoff transformation and majority rule, all of them with block size b = 2. In Section 3 we explain how to generate the low-T series for the latter example using a computer algorithm. To show the performance of the method, we construct the series for the magnetization and energy density up to 15 terms. In Section 4 the study of those RG transformations near the Ising first-order phase transition line is considered. Finally in Section 5 we present our conclusions.

2 Series Expansions for Renormalized Operators

2.1 Review of Low-T Expansions

Let us consider for simplicity a ferromagnetic Ising model on a two–dimensional square lattice. The spins take the values ± 1 and interact through the Hamiltonian

$$\mathcal{H} = -K \sum_{\langle i,j \rangle} (\sigma_i \sigma_j - 1) - H \sum_i (\sigma_i - 1) \tag{1}$$

where the first sum is over all the nearest-neighbor pairs of spins, and the second one over every point $i = (i_x, i_y)$ of the lattice. The partition function for a system of N spins with periodic boundary conditions is then

$$Z_N = \sum_{\{\sigma=\pm 1\}} e^{K \sum_{\langle i,j \rangle} (\sigma_i \sigma_j - 1) + H \sum_i (\sigma_i - 1)}$$
(2)

We have absorbed the term $\beta = 1/kT$ in the definition of the coupling constants $K \ge 0$ and H. We are mainly interested in the zero-field case (H = 0), but for future convenience we keep the second term of the Hamiltonian (1). This term will be necessary to obtain the zero-field susceptibility (see below).

The first step to compute low-T expansions is to find out the ground states of the system at T = 0. In our case it is easy to realize that when H = 0 there are only two translation-invariant ground states. Both of them are completely ordered configurations with magnetization +1 and -1 respectively. When $H \neq 0$ then there is only one ground state whose magnetization is parallel to the magnetic field H. We will choose hereafter the (+1)-state as our ground state. This implies that the magnetic field should be always non-negative $(H \ge 0)$. Furthermore, we have normalized the Hamiltonian (1) in such a way that $\mathcal{H}(+1) = 0$.

Looking at eq. (2) it is easy to realize that each flipped spin is penalized by a factor $\lambda = \exp(-2H)$ in the partition function. And each unsatisfied bond (i.e. a bond with both spins in opposite states) is suppressed by a factor $\mu = \exp(-2K)$. All the spin configurations with *n* flipped spins and *m* unsatisfied bonds give the same contribution to the partition function (2) and equal to $\mu^m \lambda^n$. So we can group these configurations together and express the partition function as

$$Z_N(\mu,\lambda) = \sum_{m,n} Z_{m,n}^{(N)} \mu^m \lambda^n \tag{3}$$

where $Z_{m,n}^{(N)}$ is the number of configurations with m unsatisfied bonds and n flipped spins that occur in the system. These numbers depend explicitly on the size of the system, as well as on the boundary conditions. The first term of the expansion corresponds to the ground state, the second to one flipped spin (n = 1, m = 4), the third to two nearest-neighbor flipped spins (n = 2, m = 6), and so on. With this choice of boundary conditions, $Z_{m,n}^{(N)} = 0$ for odd values of m. This expansion is exact for finite N if all the 2^N possible configurations are taken into account.

The low-*T* expansion of the partition function (3) contains the most relevant terms when the temperature goes to zero. It can also be viewed as an enumeration of the low-energy excitations of the system. Here we are interested in developing an expansion valid as $K \to \infty$ with *H* bounded (i.e. an expansion in powers of μ (\ll 1) whose coefficients are functions of λ) ³. Thus, the dominant terms are those with the smallest values of *m*. For a given value of *m* the possible values of *n* are finite. For excitations which do not see the boundary of the system the allowed values of *n* are given by $n \in [m/4, m^2/16] \cup [N-m^2/16, N-m/4]$ (resp. $[(m+2)/4, (m^2-4)/16] \cup [N-(m^2-4)/16, N-(m+2)/4]$) when m/2 is even (resp. odd). All the terms with the same *m*, irrespective of *n*, are considered to contribute at the same order (i.e. λ is considered to be of order 1). This feature implies that we can compute derivatives of the series expansions with respect to the magnetic field *H*. When the temperature is very close to zero only a few terms are needed to provide an accurate description of the system. However, as the temperature increases we have to include more and more terms in the expansion to attain a similar accuracy.

Actually, the partition function expansion is a technical tool to compute the expectation values of some local operators: the energy density $E = \langle \sigma_{(0,0)} \sigma_{(1,0)} \rangle$ and the magnetization $M = \langle \sigma_{(0,0)} \rangle$. The relations for a finite system are the following

$$E_N(\mu,\lambda) = 1 + \frac{1}{2N} \frac{1}{Z_N} \frac{\partial Z_N}{\partial K} = 1 - \frac{1}{N} \frac{\mu}{Z_N} \frac{\partial Z_N}{\partial \mu} = \sum_{m,n} E_{m,n}^{(N)} \mu^m \lambda^n$$
(4a)

$$M_N(\mu,\lambda) = 1 + \frac{1}{N} \frac{1}{Z_N} \frac{\partial Z_N}{\partial H} = 1 - \frac{1}{N} \frac{2\lambda}{Z_N} \frac{\partial Z_N}{\partial \lambda} = \sum_{m,n} M_{m,n}^{(N)} \mu^m \lambda^n$$
(4b)

As before, the coefficients $\{E_{m,n}^{(N)}, M_{m,n}^{(N)}\}$ do depend on the lattice size and, in general, on the boundary conditions.

Let us discuss now the thermodynamic limit $(N \to \infty)$ of these expansions. In this limit, the contribution of all the terms with the same m is not in general of the same order. In particular, for H > 0 the configurations with n near N (for instance, $n \in [N - m^2/16, N - m/4]$ for m/2 even) are exponentially suppressed, and can therefore be dropped. Moreover, for H = 0 the $\sigma \to -\sigma$ symmetry implies that the contribution of the terms with n near zero is equal to the one of those with n near N. However, at $H = 0^+$ only the first set is selected. Therefore, for H > 0 or $H = 0^+$ the correct expansion is obtained by taking all the terms with n near zero.

On the other hand, the series corresponding to the partition function (3) are meaningless when $N \to \infty$, as all the coefficients $Z_{m,n}^{(N)}$ (except for $Z_{0,0}^{(N)} = 1$) diverge in that limit. This is not true for the

³Different expansions are obtained when $H \to \infty$ and K remains bounded or when both K and H diverge with $K/H \to$ constant.

series (4a,4b) whose coefficients have a well-defined limit

$$E(\mu,\lambda) = \sum_{m,n} E_{m,n} \mu^m \lambda^n \quad ; \qquad E_{m,n} = \lim_{N \to \infty} E_{m,n}^{(N)}$$
(5a)

$$M(\mu,\lambda) = \sum_{m,n} M_{m,n} \mu^m \lambda^n \quad ; \qquad M_{m,n} = \lim_{N \to \infty} M_{m,n}^{(N)}$$
(5b)

Here it is assumed that the limit $N \to \infty$ commutes (for both quantities) with the expansion in μ and λ . This fact is necessary to identify the limiting series with the thermodynamic limits of the energy density and magnetization. The coefficients $\{E_{m,n}, M_{m,n}\}$ do not depend on the boundary conditions of the finite systems.

Finally, the specific heat C_v and the susceptibility χ are defined as follows

$$C_{v}(\mu,\lambda) = \sum_{\langle x,y\rangle} \left[\langle \sigma_{x}\sigma_{y}\sigma_{(0,0)}\sigma_{(1,0)} \rangle - E^{2} \right] = \frac{\partial E}{\partial K} = -2\mu \frac{\partial E}{\partial \mu}$$
(6a)

$$\chi(\mu,\lambda) = \sum_{x} \left[\langle \sigma_x \sigma_{(0,0)} \rangle - M^2 \right] = \frac{\partial M}{\partial H} = -2\lambda \frac{\partial M}{\partial \lambda}$$
(6b)

where the sum $\sum_{\langle x,y \rangle}$ is over all nearest–neighbor pairs of spins.

The series expansions for the zero-field case $(H = 0^+ \text{ or } \lambda = 1^-)$ can be easily obtained from the previous ones by summing over the index *n*. For example, $M(\mu) = \sum_m M_m \mu^m$ where $M_m = \sum_n M_{m,n}$. For the two-dimensional Ising model we can easily compute the corresponding zero-field expansions for the energy density, specific heat and magnetizations from the known exact solutions [17, 18, 19] and the aid of an algebraic manipulator such as Mathematica. However, the zero-field susceptibility is not exactly known. Series are available up to order $\mathcal{O}(\mu^{56})$ [16].

In this paper we are mainly concerned about the computation of expectation values of more complicated local observables O. By local operator we mean an operator which only depends on a finite number of spins. Our definitions of the energy density and the magnetization do satisfy this property. The previous procedure can be generalized to include also this case by adding to the Hamiltonian (1) a new term proportional to a translation-invariant version of the operator O.

However, this method is not feasible for very complicated operators, such as the ones considered in the next Section. In this paper we propose to use the following identity

$$\langle O \rangle = \lim_{N \to \infty} \frac{1}{Z_N} \sum_{\{\sigma \pm 1\}} O(\sigma) e^{-\mathcal{H}(\sigma)}$$
(7)

to overcome this problem. The term $\exp(-\mathcal{H})$ can be expanded in terms of configurations with m unsatisfied bonds and n flipped spins as we did in (3). In this case not all the configurations with the same values of m and n give the same contribution to the numerator of (7). This contribution is equal to $\mu^m \lambda^n$ times the value of the operator $O(\sigma)$ at the configuration. Let us consider a simple example. To compute the magnetization series one has to consider, for instance, the operator $O = \sigma_{(0,0)}$ (translation invariance assures that the mean value of this operator will coincide with the magnetization (5b)). For instance, the contribution of the one-flip configurations is different depending on whether the flipped spin coincides or not with $\sigma_{(0,0)}$. In the first case it is equal to $-\mu^4 \lambda$ and in the second one to $+\mu^4 \lambda$. The same occurs for more complicated configurations (and operators). For a finite volume we obtain in this way an expansion similar to (4a, 4b). The final result $\langle O \rangle = \sum_{m,n} O_{m,n} \mu^m \lambda^n$ is obtained after performing the thermodynamic limit.

The main advantage of this method is that it allows the computation of low-T series for arbitrary operators. Its main drawback is that we need to compute two series for each observable, not one as in the former method. Furthermore, in Section 3 it is shown that its implementation on a computer is much less efficient than the corresponding to the first procedure. Its interest relies on the fact that this method could be used to compute the expectation values of any renormalized operator.

2.2 Renormalization Group Transformations

RG transformations are usually viewed as a map in a certain space of Hamiltonians (i.e. \mathcal{B}^1). This approach has a main drawback: for some commonly used RG transformations the image Hamiltonian

does not belong to the space \mathcal{B}^1 when the original interaction is located in the vicinity of the Ising first order phase transition at low enough temperature. On the other hand, strictly local RG transformations do always exist as a map in the space of translation-invariant measures [11].

Let us consider the RG transformations from this alternative point of view. The original Ising system can be completely described by means of a probability distribution ν over its configuration space. Later on, the relationship between this measure and the Hamiltonian (1) will be discussed.

The next step is to define the renormalized spins. First we divide the whole lattice into blocks. (for simplicity we will assume here that these are 2×2 blocks). To each block B_i we associate a new (renormalized) spin σ'_i ⁴. The RG transformation is the rule which gives the $\{\sigma'\}$ configuration from the original one $\{\sigma\}$. This rule could be either stochastic or deterministic, but in any case the renormalized spin should only depend on the spins belonging to the corresponding block (strict locality condition). Mathematically speaking we give a probability kernel $T(\sigma, d\sigma')$. For each configuration of the original spins $\{\sigma\}, T(\sigma, \cdot)$ is a probability distribution for the $\{\sigma'\}$ spins and furthermore, it satisfies the property $\int T(\sigma, d\sigma') = 1$. On the other hand, it is usually assumed that T is strictly local in position space and that it maps translation-invariant measures into translation-invariant ones.

The probability distribution ν' of the image system is given by

$$\nu' = \nu T = \int d\nu(\sigma) T(\sigma, \cdot)$$
(8)

and the expectation value of any local observable in this renormalized measure can be written as

$$\langle O \rangle_{\nu'} = \int d\nu(\sigma) \left[\int T(\sigma, d\sigma') O(\sigma') \right] = \langle \tilde{O}(\sigma) \rangle_{\nu}$$
(9)

The probability kernel $T(\sigma, \cdot)$ when acting on the measure $d\nu(\sigma)$ gives a probability distribution on the new spins $\{\sigma'\}$ (i.e. a renormalized measure ν'). On the other hand, we can consider its action on the operator $O(\sigma')$. In this case the results is a composite operator $\tilde{O}(\sigma) = (T \cdot O)(\sigma)$ which depends only on the original spins. Thus, the expectation value of any local renormalized operator is equal to the mean value of a certain composite operator in the original measure.

This discussion is general: the conclusions hold whether the systems can be described or not by a Hamiltonian $\mathcal{H} \in \mathcal{B}^1$. Now we take into account the role of the Hamiltonians. Given an interaction $\mathcal{H} \in \mathcal{B}^1$ we can construct a measure over the spin configuration space using the Gibbs prescription

$$d\nu(\sigma) = d\nu^0(\sigma) \frac{1}{Z} e^{-\mathcal{H}(\sigma)}$$
(10)

For finite systems this formula gives the correct answer, but for infinite systems one has to be more careful and consider the limit of the measures for finite systems and given boundary conditions as the size of the systems goes to infinite in a given sense. In (10) $d\nu^0(\sigma)$ is the a-priori measure we assign to the space of configurations of a single spin (in our case it is just the counting measure which gives to each state a probability 1/2). For finite systems the relation between Hamiltonians and measures is one-to-one. However, in the thermodynamic limit that is not the case: one Hamiltonian can be associated to several measures (i.e. at first order phase transitions) or there are perfectly sound measures which cannot be constructed via the Gibbs prescription from any sensible Hamiltonian [11].

The Hamiltonian (1) does belong obviously to the set \mathcal{B}^1 , so we can construct the measure ν using (10). Then the expectation value (9) of any local renormalized operator can be written as

$$\langle O \rangle_{\nu'} = \langle \tilde{O} \rangle_{\nu} = \lim_{N \to \infty} \frac{1}{Z_N} \sum_{\{\sigma = \pm 1\}} \tilde{O}(\sigma) e^{-\mathcal{H}(\sigma)}$$
(11)

where the definition of $d\nu^0$ has been taken into account.

In Section 2.1 we showed how to obtain low-T expansions for a general mean value $\langle O \rangle_{\nu}$. Thus, the same procedure can be applied to (11), and series of the type $\langle O \rangle_{\nu'} = \sum_{m,n} O'_{m,n} \mu^m \lambda^n$ are obtained. The practical applicability of this method relies heavily on the actual form of the kernel T as it is shown below. This procedure can also be easily generalized to several RG steps.

⁴We will denote renormalized quantities with a prime

It is important to remark that this method does not suffer from any of the pathologies which are exhibited by the RG when we try to define it as a map from a Hamiltonian space into a Hamiltonian space. Here we have not tried to define any renormalized interaction \mathcal{H}' related with the renormalized measure ν' via the Gibbs prescription (10). Our results are independent of the Gibbsian or non-Gibbsian nature of the renormalized measure.

Let us illustrate this method with three examples:

Example 1: Decimation

This case is really simple because this transformation fixes one spin of the block to be the renormalized one. In particular, the (deterministic) kernel T takes the form

$$T(\sigma, \sigma') = \prod_{i} \delta(\sigma'_{i}, \sigma_{2i})$$
(12)

where the product is over all sites i of the renormalized system.

We are only interested in computing observables that are monomials of the spins $(O = \{\sigma_{(0,0)}, \sigma_{(0,0)}\sigma_{(1,0)}\})$. So it is enough to compute for each RG transformation the composite operator $\tilde{\sigma}_i$. In this case this is equal to

$$\tilde{\sigma}_i = \int T(\sigma, d\sigma') \sigma'_i = \sigma_{2i} \tag{13}$$

This implies that the zero-field quantities are given by

$$M'(\mu, 1^{-}) = \langle \tilde{\sigma}_{(0,0)} \rangle = M(\mu, 1^{-})$$
 (14a)

$$E'(\mu, 1) = \langle \tilde{\sigma}_{(0,0)} \tilde{\sigma}_{(1,0)} \rangle = \langle \sigma_{(0,0)} \sigma_{(2,0)} \rangle(\mu, 1)$$
(14b)

where the r.h.s. of the second equation is just the unrenormalized third neighbor correlation function. This case is trivial: the renormalized correlation functions are equal to the unrenormalized ones at twice the distance. And these functions can be obtained in the two-dimensional Ising model from the exact solution [17, 18, 19].

On the other hand, this method also allows to obtain the renormalized susceptibility and specific heat. However, they cannot be computed by using derivatives as in the usual Ising model (that is because we do not know the renormalized coupling constants H' and K', if they exist). One is forced to use their definitions (6a,6b) in terms of correlation functions. It would be very interesting to devise an algorithm to build the low-T series for such quantities to an arbitrary order.

Example 2: Kadanoff Transformation

This is given by the following (stochastic) probability kernel

$$T(\sigma, \sigma') = \prod_{i} \frac{e^{p\sigma'_{i} \sum_{j \in B_{i}} \sigma_{j}}}{2\cosh(p \sum_{j \in B_{i}} \sigma_{j})}$$
(15)

where p is a free real parameter. Then,

$$\tilde{\sigma}_i = \tanh\left(p\sum_{k\in B_i}\sigma_k\right) \tag{16}$$

The first terms can be computed by hand

$$M'(\mu, 1^{-}) = \tanh 4p - 4(\tanh 4p - \tanh 2p)\mu^{4} - 4(3 \tanh 4p - 2 \tanh 2p)\mu^{6} - (36 \tanh 4p - 4 \tanh 2p)\mu^{8} + \mathcal{O}(\mu^{10})$$
(17a)
$$E'(\mu, 1) = \tanh^{2} 4p - 8(\tanh^{2} 4p - \tanh 4p \tanh 2p)\mu^{4} - 2(11 \tanh^{2} 4p - 6 \tanh 2p \tanh 4p - \tanh^{2} 2p)\mu^{6} - (43 \tanh^{2} 4p + 40 \tanh 2p \tanh 4p - 20 \tanh^{2} 2p)\mu^{8} + \mathcal{O}(\mu^{10})$$
(17b)

The limit $p \to 0$ corresponds to the case in which the σ' are not correlated with the original spins and thus, the renormalized spins do not interact among them. For this reason both quantities are zero. The limit $p \to \infty$ corresponds to the majority rule with equally-probable tie-breaker. This case will be treated in the next section.

Example 3: Majority Rule

In this case

$$T(\sigma', \sigma) = \prod_{i} \delta\left(\sigma'_{i} - \operatorname{sign}\left(\sum_{j \in B_{i}} \sigma_{j}\right)\right)$$
(18)

When sign(·) = 0 we choose $\sigma' = -1$ or +1 with probabilities $q \in [0, 1]$ and 1 - q respectively. The composite operator $\tilde{\sigma}$ takes the form

$$\tilde{\sigma}_i = \operatorname{sign}\left(\sum_{k \in B_i} \sigma_k\right) \tag{19}$$

The first terms for general q are:

$$M'(\mu, 1^{-}) = 1 - 8q\mu^{6} - (10 + 44q)\mu^{8} + \mathcal{O}(\mu^{10})$$
(20a)

$$E'(\mu, 1) = 1 - 16q\mu^6 - (20 + 88q - 4q^2)\mu^8 + \mathcal{O}(\mu^{10})$$
(20b)

The result with q = 1/2 was first reported in ref. [11]. Notice that the $\mathcal{O}(\mu^4)$ term vanishes. This is due to the fact that one-spin excitations cannot produce any flipped renormalized spin $\sigma' = -1$.

3 Series for the Majority Rule and q = 1/2

The low-T series for this particular transformation can be improved systematically with the aid of a computer algorithm. The one used here is inspired on the Recursive Counting Method (RCM) of refs. [13, 14] where details can be found. This one consists essentially on a recursive enumeration of the most relevant configurations of the system and can be easily implemented on a computer. However, there are several differences which should be noticed.

We place the spins on a $L_x \times L_y$ square lattice with periodic boundary conditions in the *x*-direction and fixed on the other one. In particular we put cold walls of +1 spins at both vertical ends of our system. This fact automatically selects the (+1) configuration as our ground state.

The desired series for renormalized operators cannot be related in a simple way to derivates of the partition function. For our purposes it is rather useful to write (11) in the following equivalent form (for the magnetization) valid only for this RG transformation

$$M' = \langle \tilde{\sigma}_{(0,0)} \rangle = \left\langle \operatorname{sign}\left(\sum_{k \in B_{(0,0)}} \sigma_k\right) \right\rangle = \sum_{\{s_i \pm 1\}} \operatorname{sign}\left(\sum_{k \in B_{(0,0)}} s_k\right) \left\langle \prod_{j \in B_{(0,0)}} \delta_{\sigma_j, s_j} \right\rangle$$
(21)

The procedure is simple: i) Decide where to place the renormalized spin on the lattice. ii) For each configuration $\{s_i\}$ of the original spins belonging to the block $B_{(0,0)}$, compute the expectation value $\langle \prod_{j \in B_{(0,0)}} \delta_{\sigma_j,s_j} \rangle$. Notice that this expectation value should be calculated with the unrenormalized measure. iii) Finally we obtain M' using the later formula. For the renormalized energy $E' = \langle \tilde{\sigma}'_{(0,0)} \tilde{\sigma}'_{(1,0)} \rangle$ the formula is very similar, although there are two renormalized spins involved (and two blocks).

The expectation value $\langle \prod_{j \in B_{(0,0)}} \delta_{\sigma_j,s_j} \rangle$ can be obtained using the RCM. The only difference is that when we arrive at any of the spins $\sigma_j \in B_{(0,0)}$ we have to fix its value to s_j . The sum in eq. (21) contains in general 2^{4b} terms, where b is the number of blocks involved in the computation (b = 1 for the magnetization and b = 2 for the energy). This feature makes this method much slower than the pure RCM. However there is a trick which allows us to save a factor of 1.6 in CPU time. When q = 1/2, configurations with sign(·) = 0 do not have a net contribution to (21): half of the times they give some contribution and the other half, minus this one.

Another disadvantage of our procedure is that it breaks the homogeneity of the lattice. There are some special blocks $(B_{(0,0)})$ for the magnetization, and $B_{(0,0)}$ and $B_{(1,0)}$ for the energy density) which are clearly different from the rest. This feature implies that, for a given order, our method needs a larger lattice than the RCM. Here the length of the series is mainly limited by L_x : the result is exact up to order $\mathcal{O}(\mu^{L_x-2})$ whenever $L_y \geq L_x$. In our case the first statement is true, but the order $\mathcal{O}(\mu^{L_x-2})$ is achieved only if $L_y \geq 2L_x - 4$ (Here we assume that the renormalized spins are placed in the middle of the lattice⁵ and, for E' the bond which joins both spins is parallel to the x-axis). As in refs. [13, 14] we can improve the performance of the algorithm by introducing different couplings $(K_x \text{ and } K_y)$ for horizontal and vertical bonds. If we want to compute M' to order $\mathcal{O}(\mu^{2L})$ we need a lattice of size $L_y = 2L - 3$ and $L_x = (L+2)/2$ $(L_x = (L+1)/2)$ if L is even (odd). In this way we obtain half of the terms which contribute to $\mathcal{O}(\mu^{2L})$ and the rest can be recovered using the symmetry of the result under $K_x \leftrightarrow K_y$. This is not longer true for E' as the bond joining the renormalized spins distinguishes one axis from the other. To overcome this difficulty we have to run the program twice: the first time that bond is horizontal and the second one vertical. To obtain the same precision we have to use different lattice sizes. When the bond is horizontal we need a lattice with $L_y = 2L - 4$ and $L_x = (L+5)/2$ $(L_x = (L+6)/2)$ when L is odd (even). And if it is vertical, $L_y = 2L - 2$ and $L_x = (L+1)/2$ $(L_x = (L+2)/2)$.

In this way we have been able to obtain the series (5a, 5b) up to order $\mathcal{O}(\mu^{30})$. The result is displayed in Table 1. In this algorithm we need to deal with very large numbers, much larger than the precision of the computer (32 bits in our case). For that reason, we used modular arithmetic in the FORTRAN code to obtain all the coefficients. And all the series manipulation was done using Mathematica, which allows infinite-precision integer arithmetic. We checked the algorithm by reproducing the known series for the unrenormalized observables M, E and χ . With the use of more sophisticated tricks to save memory these series could be extended a lot more.

4 Study of the First–Order Phase Transition at Very Low Temperatures

For the two-dimensional Ising model some rigorous results are known about the behavior of the RG at the first-order phase transition. The authors of ref. [11] found that the renormalized measure is not Gibbsian for some particular RG transformations *at* the transition line. These are the following

- Decimation for blocks of size b = 2 and $K > (1/2) \cosh^{-1}(1 + \sqrt{2})$. For $b \ge 3$ they only could prove this statement for large enough K.
- Kadanoff transformation with $0 , block size <math>b \ge 1$, and sufficiently large K.
- Majority rule for blocks of size $b = 7, 41, \ldots$ and K large enough.
- Block-averaging transformation for even $b \ge 2$ and sufficiently large K. In this case they were also able to prove that the same conclusion is true for arbitrary magnetic field H provided K is large enough.

In actual MCRG calculations one chooses by hand a linear subspace $V_n \in \mathcal{B}^1$ of the space of sensible Hamiltonians. Then, given certain renormalized expectation values, one tries to obtain a renormalized Hamiltonian $\mathcal{H}'_n \in V_n$ in such a way that the measure constructed from \mathcal{H}'_n is similar in some sense to the true renormalized measure ν' . Most "reconstruction" methods are based in Schwinger–Dyson equations [20, 21, 22]. The idea is simple: minimize a certain functional (which depends on the method) involving both renormalized expectation values (the input) and renormalized couplings (the output). It can be shown [22] that these methods provide a unique solution \mathcal{H}'_n , which coincides with the true one \mathcal{H}' if this latter interaction belongs to the trial subspace V_n . The key property of these functionals is that they are strictly convex.

Here we will consider the procedure given in ref. [11]. It is based on the minimization of the relative density entropy with respect to the true renormalized measure ν' . This functional in also strictly convex

⁵In this way we minimize the border effects due to the cold walls

and thus, the solution is unique in each V_n . They also proved that the solution \mathcal{H}'_n should satisfy the following conditions

$$\langle O_i \rangle_{\nu'} = \langle O_i \rangle_{\nu'_n}; \qquad \forall O_i \in V_n \tag{22}$$

where ν'_n is one Gibbs measure constructed from the Hamiltonian \mathcal{H}'_n . In this case we have the same number of equations than unknown parameters. However, when we restrict these equations to a zero-field subspace it is not always possible to find a solution.

If the measure ν' is Gibbsian we expect that the sequence of solutions \mathcal{H}'_n will converge to the true (and existing) solution \mathcal{H}' . However, if the measure is non–Gibbsian the situation is less clear. It could happen that the norm in \mathcal{B}^1 of the solutions \mathcal{H}'_n will diverge as $n \to \infty$.

Remark: More generally one could choose to look for a renormalized Hamiltonian in some *affine* subspace $A_n = V_n + \mathcal{H}_0$, where \mathcal{H}_0 is some fixed element of \mathcal{B}^1 . This will be relevant for Case I below.

Using low-T expansions we can study this procedure with no much difficulty and no statistical errors. In this section we will mainly treat the majority rule transformation with q = 1/2 and block size b = 2.

Case I: $V_1 = \{H\}$

Here the subspace V_1 contains only the magnetization; so we should solve the following equation:

$$M(K, H') = M'(K, H)$$
 (23)

In this case, $\mathcal{H}'_1 = (K, H')$ is the approximate renormalized Hamiltonian chosen within the affine subspace A_1 and the element \mathcal{H}_0 is equal to the nearest-neighbor interaction $\mathcal{H}_0 = (K, 0)$. Notice that any RG transformation satisfying $M(K, 0^+) \neq M'(K, 0^+)$ is discontinuous at H = 0 when restricted to this affine subspace A_1 .

The main interest of this case relies on its connection with ref. [8], where it was claimed that eq. (23) could be used to compute numerically the leading critical exponent of the Ising DFP. They considered the Kadanoff transformation with p = 2.5, which we now know that it does not lead to any renormalized Gibbsian measure. Actually, they used a method due to Wilson [23] which allows to linearize a RG transformation near a fixed point without suffering from truncation errors. However, it is required that this fixed point possesses only one relevant operator, and in the present case there are two relevant operators at the DFP: the magnetic field and the temperature $\sim 1/K$ [4, 10].

We can repeat the same calculation using the low-T series obtained in Section 2 by generalizing them to $H \neq 0$. As a matter of fact, it is not very difficult to notice that the leading term in $1 - M(\mu, \lambda)$ comes from one-spin flips, so it is proportional to λ . On the other hand, the leading term in $1 - M'(\mu, \lambda)$ is due to two-spin flips, and thus, it is proportional to λ^2 . The final result is

$$H' = 2H + 2K - \frac{1}{2}\log 2 \tag{24}$$

This means that there is a jump $(= 2K - (1/2) \log 2)$ at the transition line as Decker *et al* obtained. Notice that the size of the discontinuity decreases as K does. However, the slope is different from theirs. The critical exponent would be y = 1 contrary to their result and the DFP prediction (y = 2).

The same can be done for the decimation transformation with b = 2. In this case everything is much simpler because

$$M(K, H') = M'(K, H) = M(K, H)$$
(25)

This implies that H' = H and there is no jump at H = 0. The most relevant exponent is not longer relevant, but marginal (y = 0), contrary to the previous results.

In summary, we have obtained very different results for the critical exponent y depending on the used RG transformation. The critical exponents do not depend on the RG transformation, so these results are a signal that this matching method cannot be applied to this particular case. On the other hand, only decimation is continuous at H = 0, although the relation between H and H' is trivial.

Case II. $V_2 = \{H, K\}$

Now our subspace contains the original interaction $(\mathcal{H} \in V_2)$. We will try to match both the energy density and the zero field magnetization with a different zero-field Hamiltonian. If this matching can be

performed, it would mean that the RG transformation is not discontinuous at the transition line (when restricted to this coupling subspace V_2). However, this does not mean that that the renormalized measure is Gibbsian. On the other hand, if the renormalized Hamiltonian \mathcal{H}' exists, it is not guarantied that the approximants \mathcal{H}'_n do not contain any odd coupling. However, as $n \to \infty$ these odd couplings should vanish because the exact RG transformation is continuous (assuming its existence).

First we define K' as the nearest–neighbor coupling such that

$$E'(K,0) = E(K',0)$$
(26)

Using the result given in Section 2 and the well-known expansion of the Onsager solution

$$E(\mu, 1) = 1 - 4\mu^4 - 12\mu^6 - 36\mu^8 + \mathcal{O}(\mu^{10})$$
(27a)

$$M(\mu, 1^{-}) = 1 - 2\mu^{4} - 8\mu^{6} - 34\mu^{8} + \mathcal{O}(\mu^{10})$$
(27b)

we find that

$$\mu' = \sqrt{2}\mu^3 + \frac{63}{8\sqrt{2}}\mu^5 + \mathcal{O}(\mu^6)$$
(28)

The magnetization M at this particular value of $\mu = \mu'$ is equal to

$$M(\mu', 1^{-}) = 1 - 4\mu^{6} - \frac{63}{4}\mu^{8} + \mathcal{O}(\mu^{9})$$
⁽²⁹⁾

and this expansion should be compared with the renormalized magnetization $M'(\mu, \lambda)$ given in Section 2. We find that

$$M(\mu', 1^{-}) > M'(\mu, 1^{-})$$
(30)

This equation means that we can give account of the observed renormalized magnetization with a system with zero field and $K' = -(1/2) \log \mu' \approx 3K - (1/4) \log 2$. This system is not in a pure phase, but in a mixed phase because the renormalized magnetization $M'(\mu, 1^-)$ is strictly smaller than $M(\mu', 1^-)$. Thus, eq. (22) is satisfied by a measure ν'_2 which is a convex linear combination of the two pure phases ν^{\pm} characterizing the two-dimensional Ising model at low temperature and $H = 0^{\pm}$ (i.e. $\nu'_2 = \alpha \nu^+ + (1-\alpha)\nu^-$ for some $\alpha \in (0,1)$).

The same game can be played with the other two RG transformations considered in Section 2. The easiest case is the decimation transformation, where conclusions can be drawn for every $K > K_c$. In the two-dimensional Ising model it is well-known that $\langle \sigma_{(0,0)}\sigma_{(1,0)}\rangle > \langle \sigma_{(0,0)}\sigma_{(2,0)}\rangle$ for $0 < K < \infty$. This implies immediately that E(K,0) > E'(K,0) and K' < K if we take into account that E(K,0) is a strictly increasing function of K. On the other hand, the renormalized magnetization coincides with the unrenormalized one (i.e. the RG flow follows the lines of constant magnetization). And $M(K,0^+)$ is also a strictly increasing function of K for $K > K_c$. Combining both pieces we obtain that $M(K',0^+) < M(K,0^+)$ for all $K > K_c$. This is so because the direction of the RG flow is reversed: it goes from low-temperature to high-temperature (K' < K). So, we have to increase the magnetic field to keep the magnetization constant, unless the magnetization at the starting point is zero. This condition is only held above the critical temperature. In summary, we cannot match the renormalized observables using a zero-field Hamiltonian along the whole first-order transition line for this RG transformation.

For the Kadanoff transformation and large (but *finite*) p the same result holds: one cannot match the energy densities and the magnetizations with a zero-field nearest-neighbor interaction. This can only be proved when p is large enough. The reason is clear: the leading term of E' is $\tanh^2 4p$ and if p is not large, then the solution of (26) does not satisfy $\mu' \ll 1$ and the low-T series for μ' are then meaningless.

For finite p we can always choose μ_0 such that for $\mu < \mu_0$ the leading term of $E'(\mu, 1)$ is dominated by a term which does not depend on μ . Then

$$E'(\mu, 1) = 1 - 4e^{-8p} + \mathcal{O}(e^{-16p}) \tag{31}$$

if we choose $\mu_0 \sim \exp(-3p)$. The solution of eq. (26) is then

$$\mu' = e^{-2p} - \frac{3}{4}e^{-6p} + \mathcal{O}(e^{-10p}) \tag{32}$$

 and

$$M(\mu', 1^{-}) = 1 - 2e^{-8p} - 3e^{-12p} + \mathcal{O}(e^{-16p})$$
(33)

which should be compared with the expansion of the renormalized magnetization for p very large and $\mu < \mu_0$

$$M'(\mu, 1^{-}) = 1 - 2e^{-8p} + \mathcal{O}(e^{-16p})$$
(34)

We find that at leading term both quantities are the same, but the next-to-leading term is different. In particular we find that $M'(\mu, 1^-) > M(\mu', 1^-)$, so we cannot match both E' and M' with a zero-field Ising interaction. This discussion is valid as long as p is large but *finite*. When p diverges the leading term of $1 - E'(\mu, 1)$ is proportional to μ^6 and we re-obtain the result for the majority rule transformation with q = 1/2.

Case III. $V_3 = \{H, K, L\}$

Now we are considering a Hamiltonian with an additional next-to-nearest neighbor term $L \sum \sigma_i \sigma_k$. First of all we have to compute the renormalized mean value of the next-to-nearest neighbor correlation function. The result for the majority rule with random tie-breaker is

$$F'(\mu,1) = \langle \tilde{\sigma}_{(0,0)} \tilde{\sigma}_{(1,1)} \rangle = 1 - 4\mu^6 - 64\mu^8 - 336\mu^{10} - 1578\mu^{12} + \mathcal{O}(\mu^{14})$$
(35)

The second step is to write down the expressions for $\langle O_i \rangle_{\nu_n}$, $\forall O_i \in V_3$. The result for zero magnetic field is

$$E(\mu,\gamma,1) = 1 - 4\mu^4 \gamma^4 - 12\mu^6 \gamma^8 - 24\mu^8 \lambda^{12} - 32\mu^8 \lambda^{10} + 36\mu^8 \lambda^8 - 40\mu^{10} \lambda^{16} + \mathcal{O}(\mu^8 \lambda^6)$$
(36a)

$$F(\mu,\gamma,1) = 1 - 4\mu^4 \gamma^4 - 16\mu^6 \gamma^8 - 36\mu^8 \lambda^{12} - 40\mu^8 \lambda^{10} + 36\mu^8 \lambda^8 - 64\mu^{10} \lambda^{16} + \mathcal{O}(\mu^8 \lambda^6)$$
(36b)

$$M(\mu, \gamma, 1^{-}) = 1 - 2\mu^{4}\gamma^{4} - 8\mu^{6}\gamma^{8} - 20\mu^{8}\lambda^{12} - 24\mu^{8}\lambda^{10} + 18\mu^{8}\lambda^{8} - 40\mu^{10}\lambda^{16} + \mathcal{O}(\mu^{8}\lambda^{6})$$
(36c)

where $\gamma = \exp(-2L)$. Now we have to find out a pair (μ', γ') such that

$$E(\mu',\gamma',1) = E'(\mu,1); \qquad F(\mu',\gamma',1) = F'(\mu,1)$$
(37)

The solution to leading term is

$$\mu' = 4\mu^2 + \mathcal{O}(\mu^4); \qquad \gamma' = \left(\frac{1}{32\mu'}\right)^{1/4} (1 + \mathcal{O}(\mu')) \tag{38}$$

This implies that $K' \approx 2K - \log 2 > 0$ and $L' \approx (5/8) \log 2 - K'/4 \approx (7/8) \log 2 - K/2 < 0$. So, as $K \to \infty$, K' and -L' also diverge. The latter relation (38) between μ' and γ' should be taken into account when computing the actual order of a given term in the expansion of the partition function $Z_N(\mu', \gamma', 1^-)$ and its derivatives. In our case, this implies that the first two excitations to the ground state are of order μ'^3 and μ'^4 respectively. We have considered here all the excitations up to order $\mathcal{O}(\mu'^6)$.

A straightforward computation leads to the next-to-leading terms of eq. (38).

$$\mu' = 4\mu^2 \left[1 - \frac{69}{16}\mu^2 + \sqrt{2}\mu^3 + \frac{17027}{512}\mu^4 + \mathcal{O}(\mu^5) \right]$$
(39a)

$$\gamma' = \left(\frac{1}{32\mu'}\right)^{1/4} \left[1 + \frac{327}{256}\mu' - \frac{3}{16\sqrt{2}}\mu'^{3/2} + \frac{144177}{131072}\mu'^2 + \mathcal{O}(\mu'^{5/2})\right]$$
(39b)

The magnetization (36c) computed at the latter solution is equal to

$$M(\mu',\gamma',1^{-}) = 1 - 4\mu^{4} - 32\mu^{8} - \frac{2689}{16}\mu^{10} + \mathcal{O}(\mu^{11}) < M'(\mu,1^{-})$$
(40)

This implies that we cannot match the renormalized expectation values with a zero-field interaction belonging to V_3 .

5 Conclusions

In this note we have shown how to compute low-temperature expansions for the expectation values of local operators computed in the renormalized measure. In particular we have analyzed three RG transformations: decimation, Kadanoff transformation with large but finite parameter p and majority rule with random tie-breaker. All of them are defined on 2×2 blocks. We have been able to compute the first terms of the series corresponding to the renormalized magnetization and nearest-neighbor two-point correlation function for all these transformations. For the majority rule case, a computer algorithm has been devised to provide those series to an arbitrary high order. The main limitation of this computational method is the huge memory needed. With the use of more sophisticated programming tricks we expect to increase the order of both series. Here they are reported up to order $\mathcal{O}(\mu^{30})$.

These results are useful as checks for MCRG computations. Another interesting point would be to devise a new algorithm to obtain the series for the renormalized susceptibility and specific heat to an arbitrary order. As explained in Section 2, these quantities are not related by simple derivatives to the partition function, and we need to use their definition in terms of sum over connected correlation functions. This feature makes their computation a more involved matter.

The main goal of this note was the analysis of the truncation issue in the Ising model. The unrenormalized system is located at the Ising first-order transition line and very low temperature $(H = 0, K \gg K_c)$. For the three transformations considered we have found that we need a magnetic field to solve the matching equations (22) when we restrict our estimated Hamiltonian to belong to a certain finite-dimensional subspace of \mathcal{B}^1 . In particular, for the decimation and Kadanoff transformations this matching cannot be performed when restricting the equations to V_2 . For majority rule, in this case the equations admit a zero-field solution but when we consider the (larger) subspace V_3 we also need a magnetic field.

So its seems that truncation in the renormalized Hamiltonian induces some spurious odd operators (we have only found non-zero magnetic fields, but there is no reason why more complicated odd operators should not appear for larger subspaces V_n). So, the RG transformations are discontinuous at the Ising transition line when restricted to some finite-dimensional subspace of the interaction space \mathcal{B}^1 .

However, these results do not clarify the interplay between truncation and non-Gibbsianness. It is known [11] that the decimation and Kadanoff transformations lead to non-Gibbsian renormalized measures when we start at low enough temperature; and in these cases we have shown that the approximate RG transformation is discontinuous. For the majority rule the situation is less clear, as it is not known the nature of the renormalized measure. The authors of ref. [11] conjectured that in this case the renormalized measure is also non-Gibbsian, but they were able to prove it only for certain special block sizes $(7 \times 7, 41 \times 41, ...)$. In any case, this model leads to a continuous approximate RG transformation for the subspace V_2 , but a discontinuous one for V_3 . It is an open question what happens for larger subspaces V_n .

It would be very interesting to find a transformation which leads to a Gibbsian measure at low temperatures. In this case we could isolate the effect of truncation from non–Gibbsianness. A systematic study of the behavior of the estimates \mathcal{H}'_n could also be useful. When the renormalized measure is Gibbsian, the odd couplings should go to zero because the transformation is in this case continuous and single–valued. If the renormalized measure is non–Gibbsian then it is not known what could happen.

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m	M'_m	E'_m	
0	1	1	
6	-4	-8	
8	-32	-63	
10	-168	-312	
12	-816	-1328	
14	-3964	-5318	
16	-19628	-21389	
18	-99120	-89806	
20	-508848	-396826	
22	-2647012	-1828884	
24	-13917848	-8690181	
26	-73827576	-42212476	
28	-394527840	-208509354	
30	-2121643804	-1043875370	

Table 1: Series expansions for the zero–field renormalized magnetization $M' = \sum_m M'_m \mu^m$ and two–point correlation function $E' = \sum_m E'_m \mu^m$. Only the non–zero contributions are displayed.