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Monte Carlo renormalisation group study of the *XY* model on a two-dimensional random triangular lattice

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Abstract. The Monte Carlo renormalisation group method is applied to discussing the nature of the phase transition of the *XY* model on a two-dimensional random triangular lattice. A line of fixed points and a non-universal phase transition have been found, in agreement with Kosterlitz–Thouless theory.

1. Introduction

The idea of quantising field theory on a random lattice has been proposed by Christ, Friedberg and Lee [1]. It has the advantages of preserving the translational invariance and Lorentz invariance of the continuous theory which are explicitly violated on the conventional regular lattice. For a theory on a random lattice, similar to the situation on a regular lattice, the scaling limit is defined as the renormalisation continuous limit of the theory. This scaling limit corresponds to one of the critical points of the system. In this paper, using the Monte Carlo renormalisation group (MCRG) method, we investigate phase transition and critical properties of the *XY* model on a two-dimensional random triangular lattice. The Hamiltonian of the *XY* model can be written as

$$\begin{aligned} H &= -\beta \sum_{\langle ij\rangle} J_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \\ &= -\beta \sum_{\langle ij\rangle} J_{ij} \cos(\theta_i - \theta_j) \qquad 0 \leqslant \theta_i < 2\pi \end{aligned} \tag{1}$$

where $\boldsymbol{S}_i = (\cos\theta_i, \sin\theta_i)$ is a spin variable defined on the ith lattice site. $J_{ij} > 0$ are the ferromagnetic interaction weights; here we assume that they are normalised, i.e. $(1/N_1)\sum_{\langle ij\rangle} J_{ij} = 1$ where N_1 is the number of links. The sum is taken over all nearest-neighbour bonds.

This model has been studied extensively for several years. The most important result is the theorem proved by Mermin and Wagner [2], which pronounces that this model cannot develop a spontaneous ferromagnetic order at any non-zero temperature. This proof can be generalised to the random lattice explicitly. So the conventional order–disorder critical phase transition is forbidden in this system. However, the correlation functions at high and low temperature which are obtained from the high-temperature expansion and the one-loop perturbation expansion, respectively, demonstrate different asymptotic behaviours. This suggests that the system should undergo

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a phase transition in spite of the absence of the ferromagnetic order. Kosterlitz and Thouless (KT) proposed an intuitive mechanism for this phase transition: the breaking of vortex pairs [3]. Under the Villain approximation, this model is equivalent to the spin wave plus two-dimensional neutral Coulomb gas system (SWCG). Treated as a SWCG model, using a renormalisation group (RG) analysis, Kosterlitz got some quantitative results for the XY model.

This model would undergo a phase transition from a high-temperature short-range correlation phase to a low-temperature long-range correlation phase. There is a fixed-point line above the phase transition point β_c. Near or above β_c, we have the critical behaviour of the correlation length

$$\xi(\beta)\sim\begin{cases}\exp\left(\frac{\nu}{\lambda}(\beta_c-\beta)^{-\lambda}\right) & \beta\leqslant\beta_c\\ \infty & \beta\geqslant\beta_c\end{cases} \tag{2}$$

where ν and $\lambda>0$. It immediately leads to the conclusion that β_c is an infinite-order phase transition point, because the scaling part of the free energy density is $f_s(\beta)\sim\xi^{-d}(\beta)$, so

$$\frac{d^n f_s(\beta)}{d\beta^n}\sim\frac{d^n\xi^{-2}(\beta)}{d\beta^n}\underset{\beta\sim\beta_c}{\sim}0 \qquad n=0,1,2,\ldots. \tag{3}$$

From (2), using a scaling argument, one can show that the susceptibility has the critical behaviour

$$\chi(\beta)\sim\begin{cases}\exp\left(\frac{\nu}{\lambda}(\beta_c-\beta)^{-\lambda}\right) & \beta\leqslant\beta_c\\ \infty & \beta\geqslant\beta_c\end{cases} \tag{4}$$

where $\gamma>0$ and satisfies the scaling law $\gamma=\nu(2-\eta(\beta_c))$, in which the universal constant $\eta(\beta)$ is the scaling dimension at β_c. On the regular square lattice, the KT theory gives the result $\lambda=\frac{1}{2}$ [4].

In this paper, we use the MCRG method on a two-dimensional random triangular lattice to find whether the non-trivial β_c exists, and what the value of λ should be.

2. MCRG method and $\Delta\beta$ function

The MCRG method is a numerical method which combines the idea of the real space renormalisation group with the Monte Carlo simulation [5]. It provides a direct way to study the critical phenomena of a system. In the real space renormalisation group method, starting from an initial Hamiltonian $H(\{S\})$, one gets a new effective Hamiltonian $H'(\{S'\})$ through the transformation

$$\exp[-H'(\{S'\})]=\sum_{\{S\}}P(\{S'\},\{S\})\exp[-H(\{S\})] \tag{5}$$

and

$$\sum_{\{S'\}}P(\{S'\},\{S\})=1 \tag{6}$$

where $\{S'\}$ is the blocked configuration which describes the mean block properties of the original configuration $\{S\}$.

Using MC simulation, one can get a series of configurations $\{S\}_i$, $i=1,2,\ldots,N$, which satisfy the canonical distribution $\exp[-H(\{S\})]$. From a given configuration $\{S\}_i$ one can get, with the RG method, a set of configurations $\{S'\}_{j_i}$, $j_i=1,2,\ldots,m$, which satisfies the distribution $P(\{S'\},\{S\}_i)$. So, according to (5), $\{S'\}_{j_i}(j_i=1,2,\ldots,m;\ i=1,2,\ldots,N)$ would satisfy the canonical distribution $\exp(-H'(\{S'\}))$. Thus the ensemble average of any physical quantity, before and after the renormalisation transformation, can be obtained from the arithmetic average on $\{S'\}$ and $\{S\}$ respectively, if N is sufficiently large.

In the MCRG method, one usually determines the so-called $\Delta\beta$ function first. Consider a block transformation which erases away all the short-distance characters of the system with a scale b ($b>1$), then after k time transformations only the characters above the scale b^k are preserved. For sufficiently large k, we define the $\Delta\beta$ function by

$$\Gamma(\beta)_{(k)}=\Gamma(\beta-\Delta\beta(\beta))_{(k-1)} \tag{7}$$

where $\Gamma(\beta)_{(k)}$ denotes any physical result after k time RG transformations and it describes the nature of the system above the scale b^k. Equation (7) is called the matching condition. It is clear that for a critical point β_c one should have

$$\Delta\beta(\beta_c)=0. \tag{8}$$

If there is only one relevant parameter, the inverse temperature β, this matching process can be demonstrated by figure 1. In figure 1, RT denotes the renormalisation trajectory, $\beta^{-1}=\beta_c^{-1}$ is the critical surface and α is an irrelevant parameter. We choose the initial Hamiltonian to be the standard form, $H(\beta,\alpha=0)$. Starting from this standard form, after some time RG transformation, the RG flow line would be attracted to the RT, and then they will leave from the critical surface along the RT (suppose $\beta\neq\beta_c$). Adjusting $\Delta\beta$, the matching condition (7) can be satisfied and the correlation lengths satisfy

$$\xi(\beta)=b\xi(\beta-\Delta\beta(\beta)). \tag{9}$$

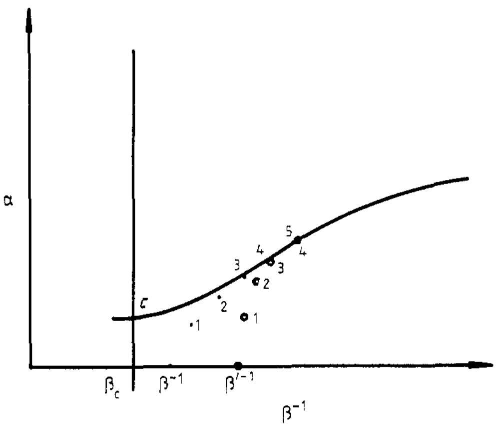

Figure 1. A matching process is illustrated in a two-dimensional coupling-constant space. The renormalisation trajectory (RT) attracts the effective Hamiltonian obtained from the standard Hamiltonian $H(\beta,\alpha=0)$ after some time RG transformations. $\beta^{-1}=\beta_c^{-1}$ is the critical surface and c is the critical fixed point. α is an irrelevant parameter.

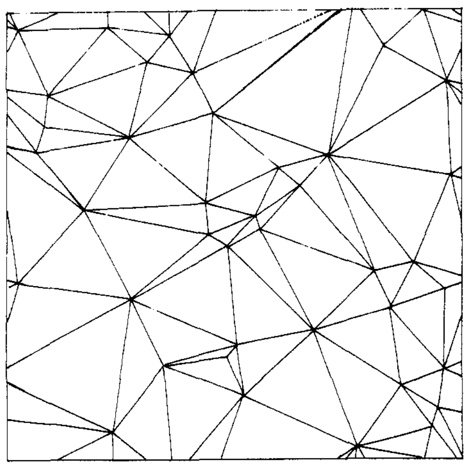

Figure 2. A two-dimensional random triangular lattice with 40 sites.

For a finite-order phase transition point β_c, the correlation length would display the asymptotic behaviour

$$\xi(\beta) \sim |\beta_c - \beta|^{-\nu}. \tag{10}$$

Thus, from (9), we get the asymptotic behaviour of $\Delta\beta$ near β_c,

$$\Delta\beta(\beta) = (b^{1/\nu} - 1)(\beta_c - \beta) \qquad \nu > 0, \beta \sim \beta_c. \tag{11}$$

For a non-trivial critical phase transition point with the asymptotic behaviour like equation (2), we have

$$\Delta\beta(\beta) = \begin{cases} \dfrac{\ln b}{\nu}(\beta_c - \beta)^{1+\lambda} & \beta \leqslant \beta_c \\ 0 & \beta \geqslant \beta_c \end{cases} \tag{12}$$

where ν and $\lambda > 0$.

So, from the asymptotic behaviour of the $\Delta\beta$ function, we can determine the value of λ and the place of β_c and thus say something about the type of the phase transition.

In the MCRG method, to diminish the effect of the finite lattice size, one usually uses the method proposed by Wilson. That is, one uses two different lattices which have similar geometric structures and linear dimensions L and L/b respectively, where b is the scale used in the RG transformation. The geometric structures of the lattices given by the k time blockings on the large lattice and $k-1$ times on the small one are identical. Thus, the matching equation should be

$$\Gamma(\beta, L)_{(k)} = \Gamma(\beta - \Delta\beta(\beta), L/b)_{(k-1)}. \tag{13}$$

In fact, the number of blocking times is limited by the finite size of the lattice (clearly, k cannot be greater than $\ln L/\ln b$). So the matching condition may not be satisfied. There are three ways to solve this problem. The first is to use a improved initial Hamiltonian, which is chosen as close to the RT as possible, instead of the standard one [6]. Another way is to use some improved observable quantities which have good low-temperature behaviour [7]. We use the third method, the improved RG transformation method [7]. Because the RT and the position of the fixed point on the critical surface are dependent on what RG transformation is used, we can choose a suitable RG transformation whose RT and fixed point are close to the initial standard Hamiltonian. Clearly, the number of transformation types which can be used is very large. We can choose a one-parameter subset in all of these RG transformations, and then find an optimal value for this parameter. In our calculation, we use the RG transformation as follows:

$$P_a(\{S'\}, \{S\}) = A \prod_{i'} \exp(a\boldsymbol{S}'_{i'} \cdot \boldsymbol{\mu}_{i'}(\boldsymbol{S}))\delta(|\boldsymbol{S}'_{i'}| - 1) \tag{14}$$

where

$$\boldsymbol{\mu}_{i'}(\boldsymbol{S}) = \sum_{i \in \omega_{i'}} \boldsymbol{S}_i \left(\left\| \sum_{i \in \omega_{i'}} \boldsymbol{S}_i \right\| \right)^{-1} \tag{15}$$

and $\omega_{i'}$ is the corresponding block. When $a \to \infty$ this transformation would become the standard blocked transformation

$$P_a(\{S'\}, \{S\}) \xrightarrow[a\to\infty]{} P_\infty(\{S'\}, \{S\}) \sim \prod_{i'} \delta(\boldsymbol{S}'_{i'} - \boldsymbol{\mu}_{i'}(\boldsymbol{S})). \tag{16}$$

The parameter a should be optimised. This can be done by setting $\Delta\beta$ to meet the scaling behaviour on the critical region, which is the low-temperature region in our case and where perturbation theory can be used if the temperature is sufficiently low.

The matching condition, when there is a free parameter a, can be written as

$$\Gamma(\beta, L, a)_{(k)} = \Gamma(\beta - \Delta\beta(\beta), L/b, a)_{(k-1)}. \tag{17}$$

Thus, on the tree diagram level, we have [7]

$$\Delta\beta(\beta) = \beta\left(1 - \frac{\alpha_{(k-1)}(L/b)}{\alpha_{(k)}(L) - \beta(b^{-2k}/a)}\right). \tag{18}$$

However, on the level of the spin-wave approximation, the $\Delta\beta$ should be zero. Thus the optimisation value of the parameter a should be

$$a = c\beta = \frac{b^{-2k}}{\alpha_{(k)}(L) - \alpha_{(k-1)}(L/b)}\,\beta. \tag{19}$$

3. The numerical results

We use two random triangular lattices which have 320 and 160 sites respectively, and satisfy the periodic boundary condition (a random triangular lattice is illustrated in figure 2). The interaction weights are set to one. The blocking procedure is as follows. We first pick out 160 sites randomly from the 320 sites of the large lattice. These 160 sites will be used as the sites of both the unblocked small lattice and the first time blocked large lattice. Then we pick out 80 sites randomly from the above 160 sites and they will be used as the sites of both the first time blocked small lattice and the second time blocked large lattice; repeating the above procedure successively, we will get the k time blocked lattice and the $(k-1)$ time blocked small one. Clearly, at any stage of the above blocking procedure, the two blocked lattices are identical in their geometric structure and the block scale factor b is $\sqrt{2}$.

The canonical ensemble averages are obtained from the Monte Carlo method. The sweep-to-sweep autocorrelation function, defined as [8]

$$\Gamma(l) = \sum_n (\Gamma(l+n) - \bar{\Gamma}) \cdot (\Gamma(n) - \bar{\Gamma})\left(\sum_n (\Gamma(n) - \bar{\Gamma})^2\right)^{-1} \tag{20}$$

is shown in figure 3. It is clear that the autocorrelation is very small after 3-5 sweeps and the independent configurations are generated by 3-5 sweeps (in the crossover region, the autocorrelation function is larger than one in the other region, but after 10 sweeps it is near to a zero). Starting from the equilibrium states which we got in another work, we perform 9000 and 7000 sweeps of heat bath iterations to get various averages on large and small lattices respectively. The statistical error in Γ is given by [9]

$$\Delta\Gamma = \sqrt{(\langle\Gamma^2\rangle - \langle\Gamma\rangle^2)/(N-1)} \tag{21}$$

where N is the number of independent configurations. In our calculations, the independent configurations are generated by 3-5 sweeps; $\Delta\Gamma$ is about 0.002. The transformation (14) is also performed using the MC method, in which a is set to be 12.5 to fit the result that $\Delta\beta = 0$ at large β.

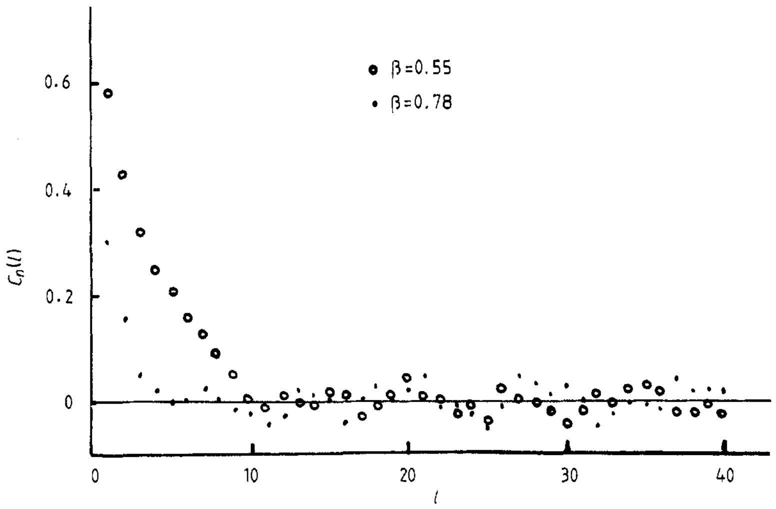

Figure 3. The autocorrelation functions for separation of sweeps at $\beta = 0.78$ and $\beta = 0.55$.

We recorded the expectation values of four different spin correlation functions as follows:

$$\Gamma_{nn}(\beta) = \frac{1}{N_1}\left\langle \sum_{\langle ij\rangle} \cos(\theta_i - \theta_j)\right\rangle_\beta \tag{22}$$

$$\Gamma_{\overline{nn}}(\beta) = \frac{1}{N_1}\left\langle \sum_{\langle \bar{i}\bar{j}\rangle} \cos(\theta_{\bar{i}} - \theta_{\bar{j}})\right\rangle_\beta \tag{23}$$

$$\Gamma_{nn\overline{nn}}(\beta) = \frac{1}{N_1}\left\langle \sum_{\langle ij\rangle} \cos(\theta_i - \theta_j)\cos(\theta_{\bar{i}} - \theta_{\bar{j}})\right\rangle_\beta \tag{24}$$

$$\Gamma_{nn^2}(\beta) = \frac{1}{N_1}\left\langle \sum_{\langle ij\rangle} \cos^2(\theta_i - \theta_j)\right\rangle_\beta \tag{25}$$

where $\bar{i}$ and $\bar{j}$ are defined as follows. The simplexes $\Delta_{ij\bar{i}}$ and $\Delta_{ij\bar{j}}$ are two triangles which take the link ij as their common edge.

The results of $\Gamma_{nn}(\beta)$ after four and three time improved renormalisation group transformations on the large and small lattices, respectively, are shown in figure 4. From these results, using the linear interpolation method and (17), we can get the values of $\Delta\beta(\beta)$ which are shown in figure 5. The other three correlation functions $\Gamma_{\overline{nn}}(\beta)$, $\Gamma_{nn\overline{nn}}(\beta)$ and $\Gamma_{nn^2}(\beta)$ reveal a similar asymptotic behaviour. Using the non-universal type $\Delta\beta$ given by (12), we found that if β_c is in the region 0.76-0.77 and λ is in the region 0.35-0.90 then it can fit in with the results of the Monte Carlo method in the asymptotic region [10]. In the KT theory $\lambda = \frac{1}{2}$.

The unblocked $-2\Gamma_{nn}(\beta)$ is just the average energy per spin, i.e.

$$E(\beta) = -2\Gamma_{nn}(\beta) = -\frac{1}{N_0}\left\langle \sum_{\langle ij\rangle} \cos(\theta_i - \theta_j)\right\rangle_\beta . \tag{26}$$

The Monte Carlo results for $E(\beta)$ which are obtained from large and small lattices respectively are shown in figure 6. It shows that the $E(\beta)$ curves are very smooth.

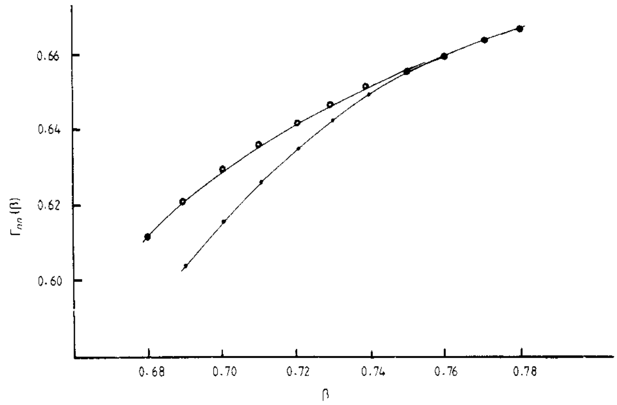

Figure 4. The results of $\Gamma_{nn}(\beta)$ after four and three time improved RG transformations on large and small lattices respectively. The results are displayed for $C = 2.5$ and $N = 320$ (●), $N = 160$ (○).

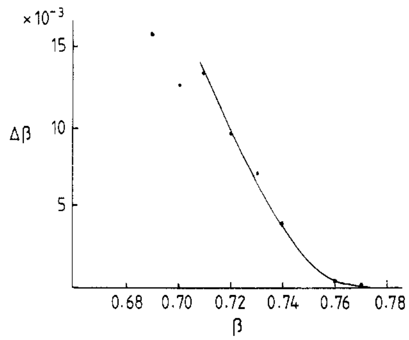

Figure 5. The $\Delta\beta(\beta)$ are obtained from the $\Gamma_{nn}(\beta)^{L}_{(4)}$ and $\Gamma_{nn}(\beta)^{S}_{(3)}$, using the linear interpolation method. The full curve shows the result of $\lambda = 0.6$ and $\beta_c = 0.77$.

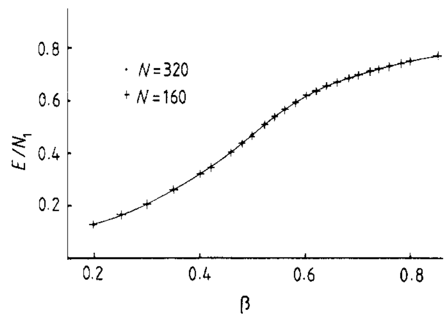

Figure 6. The Monte Carlo results of $E(\beta)/N_2$ on large and small lattices. It is clear that the shape of the energy density illustrates no size dependence. The statistical error is less than 0.002.

From figure 6 we can determine the specific heat per spin

$$c_v = -\frac{\partial E}{\partial T} = \beta^2 \frac{\partial E}{\partial \beta} \tag{27}$$

and the third or some higher-order derivatives of the average free energy per spin. With the difference technique, we can get the specific heat per spin which is illustrated in figure 7. It also shows that the peak of the c_v has no divergent tendency as the lattice size increases. It is clear that, in all the regions of β, the $E(\beta)$ and c_v obtained from two lattices with different lattice size nearly coincide with each other, it seems that the higher-order derivatives of E with respect to β could be undivergent. This fact is consistent with the conclusion we got before that $\Delta\beta$ can fit with the non-universal type of asymptotic behaviour (12).

We have also measured another two quantities on the large and the small lattices respectively, they are the susceptibility per spin $\chi(\beta)$ and the density of vortex pairs $\rho_p(\beta)$. According to the Mermin–Wanner theorem, we can write out the susceptibility

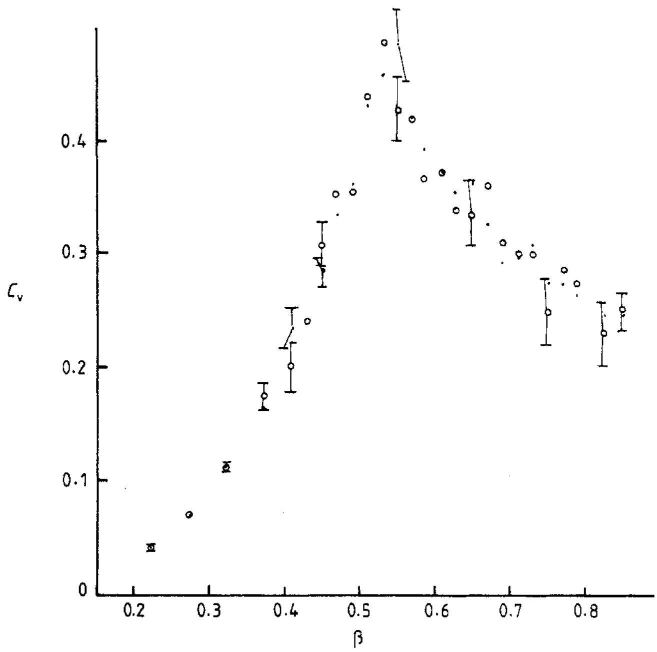

Figure 7. The Monte Carlo results of specific heat density. It also illustrates no size dependence. The diffrence of the peak of the c_v is within the limit of error.

per spin

$$\chi(\beta)=\frac{1}{N_0}\left\langle\left(\sum_i S_i\right)^2\right\rangle_\beta . \tag{28}$$

Figure 8 displays the results for $\chi(\beta)$, it is clear that in the large-β region, $\chi(\beta)$ reveals

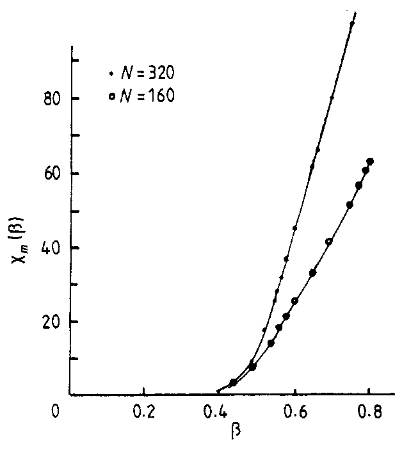

Figure 8. The Monte Carlo results of $\chi_m(\beta)$. It shows the size-dependent divergence of $\chi_m(\beta)$ in the large-β region.

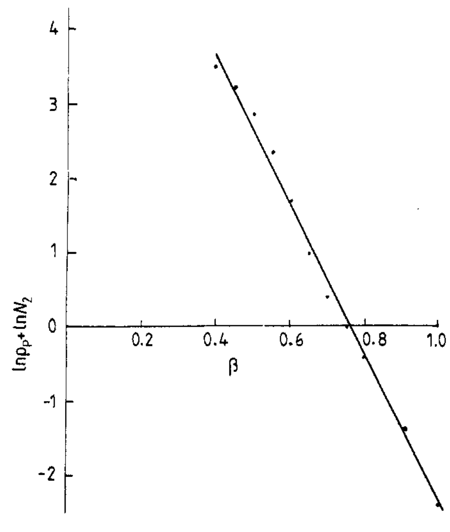

Figure 9. The logarithm of vortex pair density plotted against β for a lattice with 320 sites. The slope of the full line is -10.7.

a significant divergence tendency as N_0 increases, while in the small-β region $\chi(\beta)$ is independent of N_0.

Figure 9 is the result for $\rho_p(\beta)$, where

$$\rho_p(\beta) = \langle Q_+ \rangle_\beta / N_2 \tag{29}$$

and Q_+ is the total number of the positive vortices in a given configuration. Let Δ_{ijk} denote a two-dimensional fundamental simplex of the lattice, then Δ_{ijk} is a triangle with links $\langle ij\rangle$, $\langle jk\rangle$ and $\langle ki\rangle$ as three of its edges and x_i, x_j and x_k as its vertices, respectively, and N_2 is the number of triangles. If $\langle ij\rangle$ is a link of the lattice, then we define the multivalue angle variables Θ_i by

$$\Theta_i - \Theta_j = \theta_i - \theta_j + 2\pi I_{ij} \tag{30}$$

where $I_{ij} = 0, \pm 1, \pm 2, \ldots$ characterise the monovalue sectors of the difference $\Theta_i - \Theta_j$. Thus, the vortex number in the triangle Δ_{ijk} is defined by

$$\begin{aligned} q_{ijk} &= (\Theta_i - \Theta_j + \Theta_j - \Theta_k + \Theta_k - \Theta_i)/2\pi \\ &= I_{ij} + I_{jk} + I_{ki} \\ &= 0, \pm 1, \pm 2, \ldots\ldots \end{aligned} \tag{31}$$

In Monte Carlo simulation, we consider only the case $|q_{ijk}| \leqslant 1$. So I_{ij} can be determined by the restriction condition

$$|\Theta_i - \Theta_j| \leqslant \pi. \tag{32}$$

According to the KT theory, in the low-temperature region one should have $\rho_p \sim \exp(-2\mu\beta)$ where 2μ is the energy necessary to create a vortex pair. A plot of $\ln \rho_p$ against β is shown in figure 9. As can be seen, at low temperature $\ln \rho_p$ is proportional to β with the slope $-2\mu = -10.7 \pm 2.3$, which is consistent with the value estimated by KT of $2\mu = 10.2$ [4].

To sum up, in this paper we have studied the behaviour of the $\Delta\beta$ function of the XY model by using the Monte Carlo renormalisation group method. We obtained a fixed point line structure for the XY model on a two-dimensional random triangular lattice. We have also calculated the energy, specific heat, susceptibility and the density of vortex pairs for this model. Our results are consistent with the KT theory and the Monte Carlo results on the regular square lattice. We conclude that the XY model on a two-dimensional random triangular lattice should undergo a phase transition. This transition is an infinite-order one; the energy per spin and the specific heat per spin do not have a size-dependent behaviour. However, the susceptibility shows a clear size-dependent behaviour in the low-temperature region. This means that it should be divergent in this region. The density of vortex pairs is exponentially dependent on β.

Acknowledgment

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