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The ±J spin glass in Migdal-Kadanoff approximation

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Abstract. We study the low-temperature phase of the three-dimensional $\pm J$ Ising spin glass in Migdal-Kadanoff approximation. At zero temperature, $T = 0$, the properties of the spin glass result from the ground-state degeneracy and can be elucidated using scaling arguments based on entropy. The approach to the asymptotic scaling regime is very slow, and the correct exponents are only visible beyond system sizes around 64. At $T > 0$, a crossover from the zero-temperature behaviour to the behaviour expected from the droplet picture occurs at length scales proportional to T^{-2/d_s} where d_s is the fractal dimension of a domain wall. Canonical droplet behaviour is not visible at any temperature for systems whose linear dimension is smaller than 16 lattice spacings, because the data are either affected by the zero-temperature behaviour or the critical point behaviour.

PACS. 75.10.Nr Spin-glass and other random models

1 Introduction

There is still no agreement about the nature of the low-temperature phase of the Ising spin glass, which is defined by the Hamiltonian

$$H = -\sum_{\langle i,j\rangle} J_{ij} S_i S_j.$$

The spins can take the values ± 1, and the nearest-neighbour couplings J_{ij} are independent from each other and are most often chosen to be Gaussian distributed with mean zero and a standard deviation J.

While many Monte-Carlo simulations show properties conforming to the replica-symmetry-breaking (RSB) scenario (implying many low-temperature states and a lack of self-averaging) [1,2], other simulations [3] and analytical arguments [4] favour the droplet picture (a scaling theory based on the existence of only one low-temperature state and its time reverse). The ambiguities stem from the difficulty in reaching the asymptotic limit of low temperatures and large system sizes. Monte-Carlo results are likely to be affected by finite-size and critical-point effects. We have recently shown that a system that is known to conform to the droplet picture at sufficiently large system sizes has features similar to those of RSB if only small systems are studied and if the temperature is not low enough [5,6]. This system is the hierarchical lattice, or, equivalently, the Migdal-Kadanoff approximation (MKA) applied to a cubic or hypercubic lattice. It is thus possible that the Ising spin glass on three- or four-dimensional lattices might show its true low-temperature properties only beyond the length scales accessible to present-day Monte-Carlo simulations.

Exact evaluation of ground states and low-lying excited states appears to indicate a scenario that agrees neither with the droplet picture nor with the RSB theory, but shows instead low-lying excitations which have a fractal surface [7,8]. Newman and Stein have argued [9] that such excitations cannot give rise to new thermodynamic states. As the studied system sizes are very small, the phenomenon might be a small-size effect that vanishes at larger system sizes. Since all excitations on hierarchical lattices are combinations of compact droplets with surface dimension $d-1$ and domain walls, the MKA cannot show these low-lying excitations, and agrees with the droplet picture even for small system sizes at low temperatures with a Gaussian distribution for the bonds J_{ij}.

Very recently several papers have focussed on the $\pm J$ Ising spin glass, where the nearest-neighbour couplings take only the values 1 and -1, instead of being chosen from a Gaussian distribution [10–13]. Evidence is accumulating that the ground-state degeneracy introduces new effects. Thus, Krzakala and Martin [10] argued that even if a system showed RSB at low temperatures, different valleys in the energy landscape would differ in entropy to the extent that for sufficiently large system sizes one state would dominate the zero-temperature partition function, leading for instance to a trivial overlap distribution (*i.e.* an overlap distribution that is the sum of two δ-functions at opposite values of the overlap). This argument is supported

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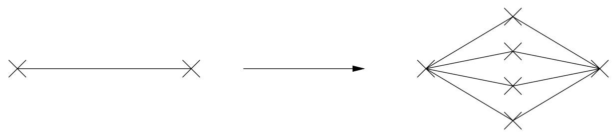

Fig. 1. Construction of a hierarchical lattice.

by simulations by Palassini and Young [11] who find a crossover from a zero-temperature behaviour with a trivial overlap distribution to a finite-temperature behaviour which seems to agree with the RSB scenario. In contrast, Hed, Hartmann and Domany, claim to find a non-trivial overlap distribution even at zero temperature [13].

It is the purpose of this paper to study the low temperature properties of the $\pm J$ model in MKA in order to shed some light on the results of Monte-Carlo simulations, and to determine the conditions under which the true low-temperature behaviour should be visible. Our findings confirm the conjecture by Krzakala and Martin that the zero-temperature behaviour is different from the low-temperature behaviour, and they also confirm the scaling assumptions concerning the entropy differences used in their argument. Furthermore, our results show that the true asymptotic zero-temperature behaviour and the true low-temperature behaviour can be seen only beyond the length scales currently studied with Monte-Carlo simulations.

The outline of this paper is as follows: In Section 2 we present our numerical results for the overlap distribution, the Binder parameter, and the recursion of the couplings within MKA. In Section 3, we give scaling arguments that yield the asymptotic exponents and the crossover behaviour seen in the simulations. Section 4 summarizes and discusses the results.

2 Numerical results

The Migdal-Kadanoff approximation is a real-space renormalization group that gives approximate recursion relations for the various coupling constants. Evaluating a thermodynamic quantity in MKA in d dimensions is equivalent to evaluating it on an hierarchical lattice that is constructed iteratively by replacing each bond by 2^d bonds, as indicated in Figure 1. The total number of bonds after I iterations is 2^{dI}. $I=1$, the smallest non-trivial system that can be studied, corresponds to a system of linear dimension $L=2$, $I=2$ corresponds to $L=4$, $I=3$ corresponds to $L=8$ and so on. Note that the number of bonds on a hierarchical lattice after I iterations is the same as the number of sites of a d-dimensional lattice of size $L=2^I$. Thermodynamic quantities are then evaluated iteratively by tracing over the spins on the highest level of the hierarchy, until the lowest level is reached and the trace over the remaining two spins is calculated [14]. This procedure generates new effective couplings, which have to be included in the recursion relations. The recursion relation of the width $J(L)$ of the two-spin coupling is for sufficiently many iterations and sufficiently low temperature given by $J(L) \propto L^\theta$, with $\theta \simeq 0.26$ in MKA in three dimensions (which is the only dimension studied in this paper).

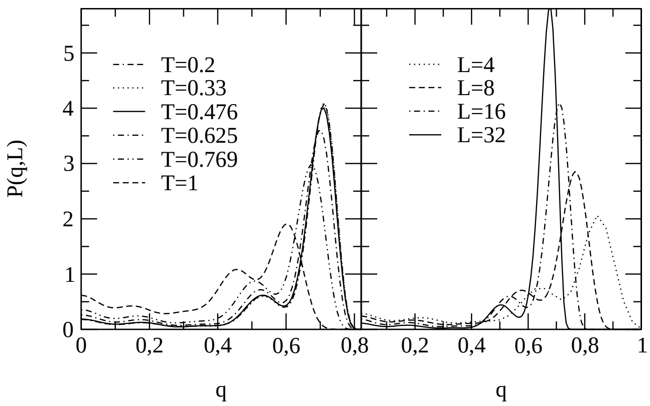

Fig. 2. The overlap distribution for the $\pm J$ spin glass in MKA for $L=16$ and $T=1$, 0.769, 0.625, 0.476, 0.33, 0.2 (left) and for $T=0.33$ and $L=4$, 8, 16, 32 (right), all averaged over several thousand samples.

We first evaluated the overlap distribution

$$P(q,L) = \left[\left\langle \delta\left(\sum_{\langle ij\rangle} \frac{S_i^{(1)}S_i^{(2)} + S_j^{(1)}S_j^{(2)}}{2N_L} - q\right)\right\rangle\right], \quad (1)$$

between two identical replicas of the system, where the superscripts (1) and (2) denote the two replicas of the system, N_L is the number of bonds of a system of size L, and $\langle ... \rangle$ and $[...]$ denote the thermodynamic and disorder average respectively. As discussed in [5], the calculation of $P(q,L)$ is made easier by first calculating its Fourier transform $F(y,L)$, which is given by

$$F(y,L) = \left[\left\langle \exp\left(\mathrm{i}y \sum_{\langle ij\rangle} \frac{(S_i^{(1)}S_i^{(2)} + S_j^{(1)}S_j^{(2)})}{2N_L}\right)\right\rangle\right]. \quad (2)$$

The recursion relations for $F(y,L)$ involve two- and four-spin terms, and can easily be evaluated numerically because all terms are now in an exponential. Having calculated $F(y,L)$, one can then invert the Fourier transform to get $P(q,L)$. Figure 2 shows our results for $L=16$ at different temperatures, and for $T=0.33$ at different system sizes respectively. Due to the ground state degeneracy, the overlap distribution for fixed L does not change below a temperature for which most samples are in the ground state. With increasing system size, the peaks in the overlap distribution become sharper, and the probability of finding an overlap value near zero decreases, indicating that one state and its spin-flipped counterpart dominate the statistics.

Figure 3 shows the probability density $P(q=0,L)$ that the two replicas have zero overlap, at several different temperatures. The two curves for $T=0.33$ and $T=0.2$ are on top of each other, indicating that at these sizes and temperatures, the system is in the ground state

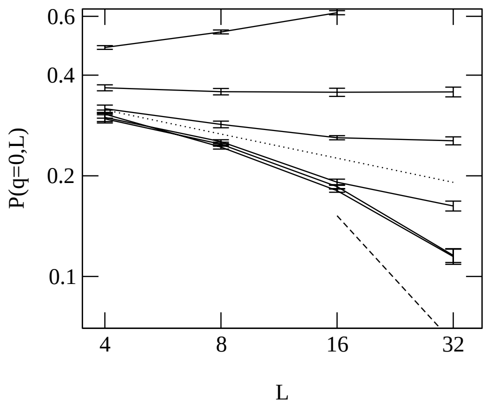

Fig. 3. The probability density $P(q = 0, L)$ for the $\pm J$ spin glass in MKA for $T = 1$, 0.769, 0.625, 0.476, 0.33, and 0.2 (from top to bottom). The critical temperature is $T_c = 1.14$. The bars indicate the standard deviation of the mean. The dotted line has the droplet picture slope $-\theta = -0.26$, which must be for sufficiently large L the asymptotic slope of all shown curves. The dashed line has the slope -1.26, which is the asymptotic slope expected for sufficiently large L at $T = 0$.

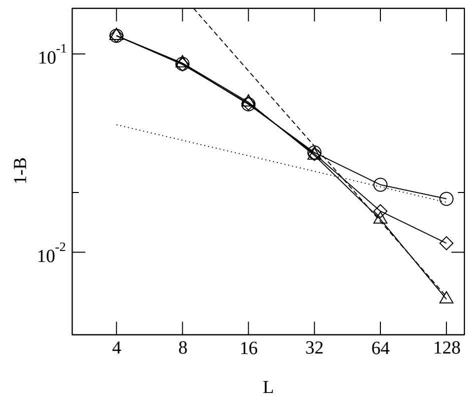

Fig. 4. The Binder parameter B as function of system size for the $\pm J$ spin glass in MKA for $T = 0.33$, 0.2 and 0 (from top to bottom). The dotted line has a slope -0.26, the dashed line has the slope -1.26. All data points are averaged over 50 000 samples.

with a probability close to 1. The $T = 0.476$ curve coincides for $L < 16$ with the $T = 0$ curve, but branches off for larger L and approaches the slope -0.26 expected from the droplet picture and seen in a system with Gaussian distributed couplings (see [5]). The $T = 0.625$ curve seems to be affected by ground state effects for $L \leq 16$, as it starts out close to the $T = 0$ curve and then has a negative slope which becomes flatter for larger L. A slope flatter than that predicted by the droplet picture indicates an influence of the critical point, as discussed in [5]. For even larger L, the curve must become steeper again and approach the slope of the droplet picture. Even the $T = 0.769$ curve appears to be affected by the ground state degeneracy for $L \leq 8$.

From these numerical results, the asymptotic behaviour of the $T = 0$ curve cannot be predicted. It seems unlikely that it becomes flatter for larger L, implying that it is fundamentally different from the droplet picture, which should govern the behaviour of a sufficiently large system at low temperatures. The asymptotic slope of the $T = 0$ curve and the crossover length scale at which a finite-temperature curve branches off from it will be derived further below. Our results also show that for system sizes smaller than around 16, all curves are affected either by the critical behaviour, or by the ground state degeneracy, so that the droplet behaviour (indicated by the dotted line in Fig. 3) is not visible for any temperature.

In order to be able to study larger system sizes, we determined the Binder parameter

$$B = \frac{3}{2}\left(1 - \frac{[\langle q^4 \rangle]}{3[\langle q^2 \rangle]^2}\right), \tag{3}$$

which can be obtained by differentiating equation (2) with respect to y. This is done by evaluating $F(y, L)$ for three small values of y. The systematic error resulting from the finiteness of y is found by evaluating $F(y)$ for a few samples for many values of y, and by extrapolating to $y \to 0$. The Binder parameter $B = 0$ in the high-temperature phase, and approaches 1 in the low-temperature phase if the overlap distribution is trivial. Within the droplet picture, $1 - B$ must scale as $L^{-\theta}$ for sufficiently large L. Figure 4 shows our results. As for the overlap distribution, the $T = 0$ curve is much steeper than the limit slope expected from the droplet picture, and the low-temperature curves branch off from it at a system size that is larger for lower temperatures. In contrast to Figure 3, system sizes can be studied that are large enough to see the differences between the three curves for $T = 0.33$, 0.2 and 0. The $T = 0$ simulation was done by taking the trace only over those configurations that contribute to the ground state, and by keeping track of the degeneracies.

Next, we tried to understand the reasons for the steep decline of the $T = 0$ curve, and of its slow approach to the asymptotic slope. For sufficiently large system sizes, the main contribution to $P(q = 0, L)$ at $T = 0$ must come from samples where a domain wall costs no energy. A domain wall is introduced into the system by flipping one of the two corner spins of the hierarchical lattice out of the ground state orientation, and by determining the new ground state resulting with this boundary condition. Samples where such a domain wall costs no energy have zero effective coupling strength $J(L) = 0$ at length scale L, with $J(L)$ resulting from the recursion relation for the width of the distribution of the couplings under the renormalization procedure. Figure 5 shows the probability of having $J(L) = 0$ (or, equivalently, of having a domain wall with zero energy cost) as function of the system size L. One can see that the slope is identical to that expected from the droplet picture beyond length scales $L = 32$, and is only slightly steeper for smaller system sizes. This indicates that the $\pm J$ model has a crossover length around 32, which is not present in the model with Gaussian distributed couplings, where the slope agrees with the droplet picture even for the smallest system sizes.

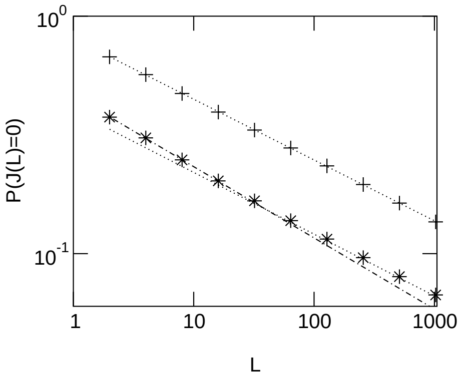

Fig. 5. The probability of having a domain wall with no energy cost in the ground state as function of the system size (* symbols). For comparison, the probability density obtained for a Gaussian coupling distribution is also shown (+ symbols). The dotted lines have the slope -0.26, the dashed line has the slope -0.3.

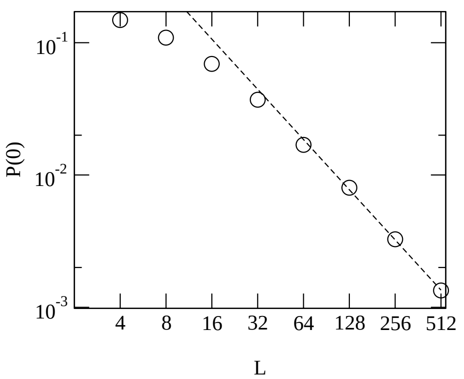

Fig. 6. The probability that the states of two replicas at $T = 0$ have a different relative orientation of their corner spins. The asymptotic slope, given by the dashed line, has the value -1.26.

Since Figure 5 agrees with the droplet picture, it cannot explain the steep decrease of $P(q = 0, L)$, and B at zero temperature. For small system sizes, not only domain walls, but also several small droplets can create a zero overlap, but this effect should become irrelevant for sufficiently large system sizes. The only remaining possibility is that while the probability for having a domain wall of zero energy agrees with the droplet picture, the weights of the two ground states with and without a domain wall differ by a factor that increases with increasing system size. In order to check this hypothesis, we evaluated the degeneracies of the two ground states that are obtained by fixing the two corner spins in parallel and antiparallel orientation respectively, and derived from this the probability that two identical replicas of the system are in the two different states. The result is shown in Figure 6. The curve is steeper by -1 compared to that of the droplet picture, indicating that entropy differences between ground states are the crucial factor causing the deviation of the $T = 0$ results from the droplet picture.

Figure 6 shows the same slow approach towards asymptopia as Figures 3 and 4. We will attempt an explanation in the next section which is devoted to a theoretical explanation of the numerical findings.

3 Scaling arguments

The main objective of the scaling theory presented here is to derive the asymptotic slope of the $T = 0$ curves, and to predict the crossover length scale at which curves at finite T branch off from the $T = 0$ curve. As shown by our numerical data presented in the previous section, entropy differences between ground state configurations that differ by a domain wall play a crucial role. Let us therefore consider a system that has a ground state for which a domain wall costs no energy, and let us estimate the order of magnitude of the entropy difference between the two ground states. One of the ground states is obtained by fixing the two corner spins of the system (those with the highest coordination number) in parallel orientation, and the other is obtained by making them antiparallel. Contributions to the entropy of each of these two states are made by droplet excitations that cost no energy. (A droplet is a block of spins that are connected to each other and that does not include one of the two corner spins, and it may comprise just a single spin). By flipping several droplets, one can thus get from every configuration contributing to one of the two ground states (with fixed corner spins) to every other configuration contributing to this state. The argument made in the following is similar to the one made by Krzakala and Martin [10] for a system with supposed RSB in the low-temperature phase. To each configuration contributing to the first ground state (with parallel corner spins), there exist configurations in the second ground state (with antiparallel corner spins) that differ from it only by a domain wall. This means that the two configurations can be transformed into each other by flipping a coherent block of spins including the right corner spin (assuming that the left corner spin is up in both states). Now, all the possible zero-energy droplets in the first configuration that do not touch the domain wall, are also zero-energy droplets in the second configuration. Droplets that do not touch domain walls can therefore make no contribution to the entropy difference between the two ground states, because they occur in both of them. The entropy difference between the two states results therefore from those droplets that touch the domain wall. Now, the domain wall involves $\propto L^{d_s}$ bonds, where d_s is the fractal dimension of the domain wall, and has the value $d_s = d-1$ in MKA. (This is because $[2^{d-1}]^I = L^{d-1}$ bonds must be cut in order to divide the system into two unconnected parts.) The average number of droplets touching the domain wall can therefore be expected to be $\propto L^{d_s}$ (assuming that the majority of droplets are small and independent from each other), and the typical fluctuation (measured over different samples, or over the two ground states) in the number of droplets touching a domain wall can be expected to be $\propto L^{d_s/2}$, which is identical to L in MKA in three dimensions.

Now, the probability that two replicas have zero overlap is proportional to the probability that a domain wall costs no energy, $\propto L^{-\theta}$, multiplied by the probability that the configurations of the two replicas have a different relative orientation of the corner spins, $\propto L^{-d_s/2}$. This explains the asymptotic slope of $-\theta - d_s/2 \simeq -1.26$ seen in Figure 6, and expected for the zero-temperature $P(q = 0, L)$ curve in Figure 3. This scaling relation for the asymptotic slope within the droplet picture was also given in [11]. For the Binder parameter, Figure 4, we expect the same asymptotic behaviour, $1 - B \sim L^{-\theta-d_s/2}$. The reason is that for large system sizes mainly samples with zero-energy domain wall excitations show a considerable difference between $\langle q^4 \rangle$ and $\langle q^2 \rangle^2$.

Next, let us discuss possible reasons why the asymptotic slope $-\theta - d_s/2$ is approached so slowly in all our plots. Our scaling argument is based on the assumption that the size distribution of the droplets that touch the domain wall does not change much with the system size. For small system sizes, the droplet size distribution might be far from the asymptotic droplet size distribution, possibly causing considerable deviations from asymptopia. This effect is probably more severe in MKA than on a three-dimensional lattice, because in MKA droplets consisting of a single spin with coordination number two make no contribution to the entropy difference between the two ground states. The reason is that flipping the domain wall transforms each spin next to the domain wall with coordination number 2 that can be flipped without energy cost (and which therefore makes a contribution to the entropy) into a spin that can be flipped only by paying the energy 4, while every spin with coordination number two along the domain wall that can be flipped only by paying energy, is transformed into a spin that can be flipped without energy cost. When the domain wall is flipped, the energy of spins in the first class changes by -2, and that of the spins in the second class by $+2$. Since the domain wall costs no energy, the numbers of the two classes of spins must be equal, and the entropy contribution due to spins with coordination number two that can be flipped without energy cost is the same for both ground states.

Furthermore, we have assumed that the fluctuation in the numbers of droplets touching the domain wall is given by the central limit theorem, which is a good approximation only for sufficiently large system sizes. Deviations from the numbers predicted by the central limit theorem may be a further reason why the asymptotic slope $-\theta - d_s/2$ is only visible for large system sizes.

Third, we have assumed that domain walls make the main contribution to $P(q = 0, L)$. This assumption is not correct for small system sizes, where droplet excitations that do not involve the corner spin may also add up to an overlap value of zero.

Finally, let us determine the crossover length scale beyond which the droplet picture should become visible for small nonzero temperatures: Within the droplet picture, we have $P(q = 0, L) \sim TL^{-\theta}$, while we have at zero temperature $P(q = 0, L) \sim L^{-\theta-d_s/2}$. A crossover between the two regimes occurs when the two quantities are equal, *i.e.*, when $L \sim T^{-2/d_s}$.

4 Conclusions

In this paper, we have studied the $\pm J$ Ising spin glass within MKA. We have found that the zero-temperature behaviour is fundamentally different from that at low temperatures, due to entropy differences between ground states. Only for length scales larger than of the order T^{-2/d_s} does the expected droplet-picture behaviour become visible. We have presented a scaling theory that predicts the asymptotic scaling exponent $-\theta - d_s/2$ for the overlap distribution at zero temperature, and we have shown from numerical results as well as from analytical arguments that the approach to this asymptotic scaling might be slow.

Our findings shed some light on recent Monte-Carlo simulations of the three-dimensional $\pm J$ Ising spin glass. While the scaling arguments by Krzakala and Martin [10] predict a decrease of $P(q = 0, L)$ at zero temperature at least with an exponent $-d_s/2$ (if one assumes with them that the system shows RSB, implying $\theta = 0$), which lies somewhere between -1.1 and -1.3, the best Monte-Carlo simulations find only a value around -0.9 [11,15]. Other Monte-Carlo simulations giving a considerably smaller exponent probably do not sample the ground state configurations with the appropriate weights (see the comment by Marinari *et al.* [16] on the simulations by Hatano and Gubernatis [17], and the remarks by Palassini and Young [11] on the simulations by Hartmann [18].) Our findings of a surprisingly slow approach to the correct asymptotic scaling can reconcile the Monte-Carlo results with the predictions by Krzakala and Martin, and also with our predictions based on the droplet picture (where the asymptotic exponent is around -1.4 or -1.5), which we believe to be the correct description of the spin-glass phase.

Our results in Figure 3 show also that for not too low temperatures the overlap distribution data may at first (for the smallest L values) be affected by the ground-state degeneracy (as indicated by a slope that is initally steeper than for larger L), then (for somewhat larger L) by the critical point (manifesting itself in a pretty flat slope), and only for sufficiently large L (which may be beyond the reach of Monte-Carlo simulations) the correct asymptotic slope given by the droplet picture. Given such a complicated behaviour, the predictions in [13] and [11] for the asymptotic behaviour of $P(q, L)$ based on small system sizes and assuming simple scaling forms have no convincing basis.

We conclude that it is possible that the $\pm J$ Ising spin glass in three dimensions and for system sizes smaller than approximately 16 does not show the correct asymptotic scaling behaviour at any value of the temperature. It remains to be seen whether the Ising spin glass with a Gaussian bond distribution has also finite-size effects which make it impossible to see even at low temperatures the correct asymptotic scaling behaviour for the system sizes presently used in computer simulations.

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