Numerical Study on Aging Dynamics in the 3D Ising Spin-Glass Model.
I. Energy Relaxation and Domain Coarsening

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Using Monte Carlo simulations, we have studied the relaxation of energy of the three-dimensional Ising spin-glass model in aging process. Our finite-size-scaling analysis on the isothermal energy decay after the quench suggests strongly that the energy relaxes by coarsening of domain walls in agreement with the droplet theory. We have also evaluated relaxation times required for spin configurations in small systems, which are regarded as isolated droplets, to flip globally. The results support the fundamental assumption of the droplet theory that coarsening of domain walls, in case of spin glasses, is driven by successive nucleation of thermally activated droplets.

KEYWORDS: spin glass, slow dynamics, aging, droplet theory

§1. Introduction

In recent years off-equilibrium dynamics, particularly aging dynamics, of spin glasses has attracted much attention theoretically, numerically and experimentally. Many experiments have confirmed that the response to small dc/ac magnetic field after quenching the system below the spin-glass transition temperature $T_c$ shows aging effects persistently at least up to the largest possible time scale available in laboratories. On the side of theories, one of the most notable advances is the analytical theory based on solvable mean-field spin-glass models, which has provided non-trivial predictions on aging effects.

Presumably one expects that the slow relaxation is caused by some underlying collective spin excitations in the system. In the case of ordering processes in non-random systems like the conventional Ising ferromagnet, the relaxational dynamics after quenching the system below the phase transition temperature is related to coarsening of domain walls which separate ordered domains of two different pure states. The typical size of the domains, $R(t)$, at time $t$ usually grows by a certain power law. This behavior can be directly studied, for instance by scattering experiments. The intriguing question is if such a picture of the coarsening of domain walls also holds for aging processes in spin glasses. Obviously, the above mentioned mean-field theory, which is exact only in infinitely large dimension, is not helpful in this respect. The domain picture based on the so-called droplet theory has provided an interesting phenomenology. However the pure states of spin glasses cannot be found in practice which makes it difficult to rationalize the domain picture in a direct way.

In the present study, we mainly focus on the energy relaxation in the 3-dimensional EA spin-glass model during the aging process simulated by Monte Carlo dynamics. The latter starts from arbitrary initial configurations at temperature $T$ below $T_c$ which simulates instantaneous quench to $T$ from $T = \infty$. We have found that the relaxation of energy can be explained consistently in terms of coarsening of domain walls as in the case of usual phase ordering processes in non-random systems. Let us briefly describe the idea here. Suppose a system is aged by elapsed time $t$ after the quench, and a typical size of domain walls has grown to $R(t)$. In the presence of domain walls, the energy per spin, $e_T(t)$, is larger than the equilibrium energy $e_T(\infty)$ at temperature $T$ by an amount

$$\delta e_T(t) = e_T(t) - e_T(\infty) \propto \frac{\Upsilon(T) (R(t)/l_0)^\theta}{(R(t)/l_0)^\delta}. \quad (1.1)$$

with $l_0$ being a certain microscopic unit of length. Here the numerator on the right-hand side is the domain wall energy where $\Upsilon(T)$ is the stiffness constant and $\theta$ is the characteristic exponent. The denominator is the volume of a domain with $d$ being the dimension of the space.

We have studied systematically the energy per spin on relatively small system sizes $L$ and at relatively higher temperatures in the spin-glass phase. This enables us to see the behaviors of two time regimes within our computational time window: the size-independent behavior of domain growth in the dynamic regime $R(t) < L$ and the size-dependent equilibrium behavior in the static regime $L < R(t)$. It has turned out that the simulated data including in the crossover region between the two regimes can be concisely described by a finite-size-scaling (FSS) function. By multiplying eq. $(1.1)$ by a scaling function $\delta e(R(t)/L)$, the scaling ansatz is proposed as

$$\delta e_T(t) = \Upsilon(T) \left( \frac{R(t)}{l_0} \right)^{\theta-d} \delta e \left( \frac{R(t)}{L} \right). \quad (1.2)$$

with $R(t) = t^{1/z(T)}$. The FSS analysis allows us to obtain the characteristic exponent $\theta$ for the domain wall energy.
The value of $\theta$ turns out to be nearly equal to the result
by Bray and Moore at $T = 0$. These results strongly
support that the aging process in the present spin-glass
model is described well in terms of coarsening of domain
walls, i.e., the droplet picture.

As described just above the FSS analysis on the en-
ergy relaxation yields the power-law growth in $t$ of the
typical domain size $R(t)$ with the exponent $z(T)$, which
is consistent with that obtained by the previous num-
erical studies using replica-overlap.\footnote{[1][3][4][3]} We have also
performed analysis on the replica-overlap with greater
statistical accuracy, and have established the consistency
between the two analyses.

A fundamental assumption of the droplet theory on
aging processes\footnote{[4]} is that coarsening of domain walls,
in case of spin glasses, is driven by successive nucle-
ation of thermally activated droplets. In order to test
this assumption, we have studied largest relaxation times
$\tau_L(T)$, which are those needed for a global spin-flip in
each sample with relatively small sizes $L$. We have found
that the $L$-dependence of $\tau_L(T)$ is consistent with the
growth law of domains, i.e., $R(t \sim \tau_L(T)) \sim L$. Fur-
thermore, the temperature dependence follows in fact an
Arrhenius law.

In our simulated results, however, there remain some
discrepancies with the original droplet theory. Firstly, it
is assumed to grow as $L^6$ in the droplet theory, while
the barrier free energy simulated grows logarithmically
with $L$. This results agree with the previous conjectures
extracted from the $t$-dependence of $R(t)$.\footnote{[3][4][3]} Secondly,
the width of the distribution of the barrier free energy
does not increase with $L$.

The present paper is organized as follows. After de-
scribing the model and numerical method in the next
section, we present and discuss the results of our sim-
ulation in §3. Section 4 is devoted to the concluding
remarks on the present work.

\section{Model and Numerical Method}

We carry on simulations on the 3D EA Ising spin-glass
model with nearest-neighbor interactions \{$J_{ij}$\} defined
by the Hamiltonian,
\begin{equation}
H = - \sum_{(ij)} J_{ij} S_i S_j,
\end{equation}
on an $N = L \times L \times L$ simple cubic lattice. The periodic
boundary conditions are adopted. The quenched random
interaction \{$J_{ij}$\} are drawn from a Gaussian distribution
with zero mean and variance one. It has been reported
that this model has a spin-glass ordered phase below the
critical temperature $T_c$ whose most recent value is re-
ported as $T_c = 0.95 \pm 0.04$\footnote{[3]} We use the single-spin-flip
heat-bath Monte Carlo method. As a unit time, which
we call one Monte Carlo Step (MCS) hereafter, we adopt
the time in which $N$ spins are updated.

The energy per spin $e_T(t)$ at $t$ MCS after the tem-
perature quench is calculated as
\begin{equation}
e_T(t) = \frac{1}{N} \sum_{\tau=1}^{t+ta} \frac{1}{2ta + 1} H(\tau),
\end{equation}
where $H(\tau)$ is a value of Hamiltonian at $\tau$ MCS. In order
to reduce thermal fluctuations we take here an average
over short time $2ta + 1$ around $t$ with $ta = t/1000$. The
average over $N$, Monte Carlo runs with independent realiza-
tions of quenched random variables \{$J_{ij}$\}, initial spin configurations, and random
numbers. We have simulated systems with relatively
small sizes ($L = 4 \sim 10$) in order to study the crossover
between the dynamic and static regimes as mentioned in
§1, as well as large systems with $L = 24$ and 32 in order
to obtain bulk behavior which is not affected by finite
size effects within our time window ($10^6$ MCS).

Following the previous works\footnote{[4][3][3]}, the length scale
of ordered domains $R(t)$ is estimated by analyzing the
replica-overlap function, $G(r, t)$, defined as
\begin{equation}
G(r, t) = \frac{1}{N} \sum_{i=1}^{N} \left[ S_i^{(\alpha)}(t) S_i^{(\beta)}(t) S_{i+r}^{(\alpha)}(t) S_{i+r}^{(\beta)}(t) \right]_{av}
\end{equation}
Here $\alpha$ and $\beta$ are indices of the two replicas which have
different random spin configurations at $t = 0$ (an instant
of the temperature quench), and are updated indepen-
dently. Its correlation length is considered to be propor-
tional to $R(t)$. In eq. (2.3) $r$ is a spatial distance which
we take only along the directions of the lattice axes. We
have simulated large systems with $L = 24$ and 32 in this
analysis.

\section{Results and Discussions}

\subsection{Finite-size scaling of $e_T(t)$}

Let us begin with analysis on the relaxation of the energy
per spin $e_T(t)$ of large systems with $L = 32$
and 24 after the quench. The log-log plots of \(\delta e_T(t) \equiv
\delta e_T(t) - e_T^{(\infty)} \) vs. $t$ are shown in Fig. 1, where $e_T^{(\infty)}$ denotes
\(\lim_{t \to \infty} \lim_{L \to \infty} e_T(t)\). We fitted the data to the
following formula\footnote{[4]}
\begin{equation}
\delta e_T(t) \equiv e_T(t) - e_T^{(\infty)} = ct^{-\lambda(T)},
\end{equation}
with $e_T^{(\infty)}$, $c$ and $\lambda$ being the fitting parameters. From
eq. (1.1) with $R(t) \propto t^{1/z(T)}$ we obtain
\begin{equation}
\lambda = (d - \theta)/z.
\end{equation}
As seen in Fig. 1, the fitting works very well. The values
of exponent $\lambda$ depend on temperature. It is propor-
tional to $T$ at low temperatures in agreement with the previous
work\footnote{[4]} Below we determine $z(T)$ and check eq. (1.2)
numerically.

In Fig. 2 we show the log-log plot of $\delta e_T(t)$ vs. $t$ at
$T = 0.7$ for small systems with $L = 4, 5, 6, 7$. It is seen
that there exist two time regions of the relaxation curves.
In the shorter time region the curves have no size depen-
dence (the dynamic regime), while in the longer time
region the curves depend on $L$ and $e_T(t)$ approaches to
an equilibrium value $e_T^{(L)}$ which also depends on $L$
(the static regime). The crossover between the two regimes
is expected to occur when a typical size of ordered domain
$R(t)$ reaches $L$. We therefore have tried some finite-size-
scaling (FSS) analyses based on eq. (1.2). It has turned
the following asymptotic limits:
\[ e_T(t) - e_T^{(\infty)} = \begin{cases} \frac{\Gamma_n(t)}{\Gamma^*(t)} \left( \frac{\tau}{L^z(T)} \right)^{\theta - d} & \text{for dynamic regime,} \\
\Gamma_n(t) \left( \frac{\tau}{L^z(T)} \right)^{\theta - d} & \text{for static regime,}
\end{cases} \tag{3.5} \]

with \( R(t) \) being proportional to \( t^{1/z(T)} \).

In practice, we have performed the above FSS fit in the following way. By making use of \( e_T^{(\infty)} \) evaluated above using the bulk data, and expecting that \( \delta e_T(t) \) varies as a function of \( x = \log t \) and \( y = \log L \), we fitted the data of \( \delta e_T(t) \) to eq. (3.3) by means of the following trial function with ten parameters,
\[ \log(e_T(t) - e_T^{(\infty)}) = (\theta - d) \log L + \log \hat{f}(t/L^z(T)) \tag{3.6} \]
\[ \simeq (\theta - d)y + \sum_{n=0}^{7} \frac{c_n}{n!} (x - z(T)y)^n \tag{3.7} \]

Here we have expanded \( \log \hat{f} \) with respect to logarithm of its argument up to the seventh order. The above fitting has been done for 10 independent \( e_T(t) \), each of which is obtained by averaging over \( N_s/10 \) samples. We have then estimated errors of exponent \( \theta \) and \( z(T) \) from its variance over the 10 independent values.

The results of the above FSS are shown in Fig. 3. We see that the scaling works quite satisfactorily. The similar results are obtained also at \( T = 0.8 \), for which we have examined systems with \( L = 4, 6, 8, 10 \) and \( N_s \) up to 130000. The exponents obtained are listed on Table I for \( \theta \) and Table II for \( z(T) \). The values of \( z(T) \) are consistent with those extracted from \( R(t) \) in the larger systems, as will be discussed in the next subsection. We therefore consider that the present FSS with eqs. (3.3) and (3.4) is quite reasonable. The exponent \( \theta \) seems almost independent on temperature as expected. Actually, its values derived by the present FSS at \( T = 0.7 \) and 0.8 are almost equal to the droplet exponent \( \theta = 0.19 \pm 0.01 \) extracted from the defect energy analysis at \( T = 0 \) by Bray and Moore.\[ ] This result in the dynamic regime confirms the domain coarsening picture described in §I.

![Fig. 1. The power law decay of excess energy per spin \( \delta e_T(t) \) in the dynamic regime. The constants \( e_T^{(\infty)} \) are obtained by fitting the simulated data to eq. (3.3). The data are at \( T = 0.4, 0.5, 0.6, 0.7, 0.8 \) from top to bottom. The systems simulated are with \( L = 32 \) and \( N_s = 1600 \) for \( T = 0.8 \) and 0.7, and with \( L = 24 \) and \( N_s = 3200 \) for \( T = 0.6 \sim 0.4 \). They are sufficiently large to obtain size-independent (bulk) energy decay.](image1)

![Fig. 2. The decay of excess energy per spin \( \delta e_T(t) \) for systems with \( L = 4 \) (circles), 5 (triangles), 6 (squares), 7 (solid circles), and 32 (solid triangles). The asymptotic energy per spin \( e_T^{(\infty)} \) is determined as \(-1.66204\) by fitting data of \( L = 32 \) to eq. (3.3). The sample numbers \( N_s \) are \( 10^5 \) for \( L = 4, 5, 6 \) and \( 3.5 \times 10^5 \) for \( L = 7 \), and 640 for \( L = 32 \).](image2)

![Fig. 3. The scaling plot of \( \delta e_T(t) \) versus \( t/L^z(T) \).](image3)
It is worth noting that static energy of finite size systems is higher than that of the infinite one by an amount \( L^\theta \), that is,

\[
\left( \frac{L}{L_0} \right)^d e_T(t) = \left( \frac{L}{L_0} \right)^d e_T^{(\infty)} + \frac{\theta}{2} \left( \frac{L}{L_0} \right)^2.
\]  

This is interpreted that the imposed periodic boundary conditions distort the spin correlations with respect to what would be realized in an infinite system. A similar and more transparent situation can be seen in a pure ferromagnet with the anti-periodic boundary condition. The latter induces competition or frustration in the loop of the interactions winding the whole system. Clearly it leaves a domain wall even in equilibrium. The FSS of eqs. (3.3) and (3.4) works well also for this case and the well known exponents, \( z = 1/2 \) and \( \theta = d - 1 \) are deduced. The situation in the present spin-glass model is more complicated since we cannot separate the effects of frustrations in bulk and of the constraint by the boundary conditions. However, the near agreement of the exponents \( \theta \) at \( T = 0.7 \) and \( 0.8 \) with the one at \( T = 0 \) suggests that the periodic boundary condition alone introduces a ‘defect energy’ similar to the one at \( T = 0 \) discussed by Bray and Moore. In this respect let us note that a similar algebraic size dependence of finite size correction to the ground state energy with the periodic boundary condition has been reported recently.

3.2 Domain growth after quench

Here we examine the replica-overlap function \( G(r, t) \) of eq. (2.3) and the domain growth \( R(t) \) after the quench. Our analysis follows the work of Kisker et al. \[14\]. We use an improved method of evaluating \( R(t) \) from \( G(r, t) \) as explained below. Because of the periodic boundary conditions, relation \( G(r, t) = G(L - r, t) \) holds, and so \( R(t) \) is evaluated as

\[
R(t) = 2 \frac{L}{2\pi} \sqrt{G(0, t)/G(2\pi/L, t)} - 1, \tag{3.9}
\]

where

\[
G(k, t) = 2 \int_0^{L/2} G(r, t) \cos kr dr. \tag{3.10}
\]

If \( G(r, t) \) is simply proportional to \( \cosh[2(r - L/2)/R(t)] \) (or \( \exp(-2r/R(t)) \) in the limit \( L \rightarrow \infty \)), the estimation of eq. (3.3) gives \( R(t) \) exactly. We consider that our estimation of \( R(t) \) is superior to the method based on the moments \( \int_0^{L/2} r^n G(r) dr \) with \( n = 0, 1 \) used by Kisker et al. since our estimation significantly reduces the irrelevant contribution from small \( r \) which deviate from an exponential law.

The averaged domain size \( R(t) \) estimated from eqs. (3.9) and (3.10), and shown in Fig. 4, are well fitted to \( R(t) = b T^{1/z(T)} \). The obtained exponents \( z(T) \) are 7.86(3), 8.71(3), 9.84(5), 11.76(6) and 14.80(7) at \( T = 0.8, 0.7, 0.6, 0.5 \) and 0.4, respectively. These values at \( T = 0.8, 0.7 \) listed on Table II are in good agreement with those extracted from the FSS analysis on \( \Delta e_T(t) \). The temperature dependence of \( z(T) \) is given by \( 1/z(T) \propto 0.17 T \) at \( T < 0.7 \). This linear \( T \)-dependence of \( 1/z(T) \) is consistent with the results by Marinari et al. \[15\] and those by Kisker et al. \[14\] though its coefficient 0.17 is different from the one estimated from those of Kisker et al.

The replica-overlap function \( G(r, t) \) is well scaled when it is plotted against \( r/T^{1/z(T)} \) as shown in Fig. 5. Furthermore it is seen that \( G(r, t) \) in a longer length scale decays in a simple exponential form. The exponents \( z(T) \)

![Fig. 4.](image1)

**Table I.** Exponent \( \theta \) evaluated by our finite-size-scaling (FSS) analysis on the energy relaxation.

| \( T \) | FSS | Bray and Moore |
|---|---|---|
| 0.8 | 0.20(2) | — |
| 0.7 | 0.19(3) | — |
| 0.0 | — | 0.19(1) |
used in this plot are those extracted by the fit of $R(t)$.

### 3.3 Distribution of barrier free-energy of isolated droplets

As mentioned in §1, another important purpose of the present work is to study directly relaxational dynamics of droplets. Since, however, it is hard to specify each droplet in bulk, we examine here characteristic time scales $\tau_L(T)$ for spin configurations of systems with small $L$ to turn over as a whole in equilibrium. We regard such systems as isolated droplets of size $L$.

At first, $t_0$ MCS is elapsed starting from a random spin configuration. Then the spin configuration $\{S^{(\alpha)}(t_0)\}$ is copied to another replica $\beta$ and the two replicas are updated independently with different sequence of random numbers. The latter is continued until the clone-number. The latter is continued until the clone-number.

In Fig. 6 we show distribution of the logarithmic times

$$P_L(\ln \tau_i), \text{ where } \tau_i = t_i - t_{i-1} \text{ with } t_0 = 0.$$ 

One can see clearly that $P_L(\ln \tau_2)$ and $P_L(\ln \tau_3)$ coincide with each other, but it is not the case for $P_L(\ln \tau_1)$. The result is interpreted that $P_L(\ln \tau_1)$ is affected by off-equilibrium effects, while $P_L(\ln \tau_2)$ can be regarded as an equilibrium distribution which we analyze in detail below with $\tau_L(T) = \tau_2 (= \tau)$. In this analysis we have examined both the periodic and free boundary conditions.

In Fig. 7-(a) we show the log-log plot of $P_L(\ln \tau)$ versus $\tau$ of the system with $L = 4$ at $T = 0.8, 0.7, 0.6$ and 0.5. If the relaxation process is of the Arrhenius-type, i.e., $\tau = \tau_0 \exp(B/T)$, the distribution of the free-energy barriers $\Phi_L(B)$ is written as

$$\Phi_L(B) = \frac{1}{T} P_L(\ln \tau/\tau_0)$$

(3.12)

where $\tau_0^{-1}$ is the attempt frequency. With $\tau_0 = 1$ the data in Fig. 7-(a) lie top on each other as shown in Fig. 7-(b). This result indicates that the relaxational dynamics of present interest is in fact an Arrhenius type whose barrier free energy $B$ little depends on temperature.

Making use of relation $B = T \ln \tau$ confirmed above, we next examine the $L$-dependence of $\Phi_L(B)$. In Fig. 8 we show the plot of $\Phi_L(B)$ against $B - B_L$ at $T = 0.8$, where $B_L$ is the value, at which $\Phi_L(B)$ is maximum for each $L$. The resultant $B_L$ is well fitted to

$$B_L = \Delta' \ln L,$$

(3.13)

as shown in Fig. 9 below. Another interesting observation in Fig. 8 is that the shape of the distribution $\Phi_L(B)$ does not depend on $L$, while its peak position does. This is certainly in disagreement with the original droplet theory in which the width of $\Phi_L(B)$ is conjectured to be of the same order as that of its mean. If the coarsening process of domains represented by $R(t)$ analyzed before is also assumed due to nucleation of domains of the corresponding size by thermally activated process, the associated barrier free energy $B_R$ is given by

$$B_R = \Delta \ln R.$$  

(3.14)

In Fig. 9 we plot $B_R$ thus evaluated and $B_L$ of eq. (3.13) against the properly scaled length $l$. For $B_R$ we set $l = 2R(t)$, while for $B_L$ we use $l = L/(2^{1/\delta})$ since the clone-correlation function can cross zero when a half of spins in the system turns over. The logarithmic dependence on $l$ of both $B_R$ and $B_L$ is clearly seen in the figure. Also it is seen that the coefficient $\Delta$ for $B_R$ is a little larger than $\Delta'$ for $B_L$. This difference may indicate that dynamics of ordered domains in a large system is not perfectly independent from their neighboring ones as was assumed in the original droplet theory. A similar conclusion has been also deduced experimentally.
3.4 Discussions

Here let us comment on the magnitude of energy, length and time scales in the aging process simulated so far. Our result is consistent with $F_L \sim L^\theta$, while the barrier free energy $B_L$ associated with them is proportional to $\ln L$. It is then naturally expected that the latter is overcome by the former at a certain value of $L$, and so that the present results cannot provide us a proper picture in the thermodynamic limit. But we note that $F_L$ evaluated from the present simulation is given by

$$F_L \propto N\delta e_T \simeq 2.0 \times (L/l_0)^\theta,$$

with $\theta = 0.19$, where the factor 2.0 is determined from the saturated value in the scaling plot of Fig. 3. Because of this small value of $\theta$, combined with a relatively large value of $\Delta (\simeq \Delta')$ in eq. (3.14) which in turn is due to a relatively large value of $z(T)(\simeq 8 \sim 10)$, $F_L$ and $B_R$ (or $B_L$) become of the same order of magnitude only when $L$ is of the order of $10^8 \sim 10^9$ with $l_0 = 1$. The corresponding time scale, for $R(t)$ to reach to this length scale, is much more than an astronomical one. In this context, it is pointed out that $B_R$ experimentally extracted by Joh et al. recently is consistent with the simulated results expressed by eq. (3.14) (with $\tau/\tau_0 \sim 10^{12}$ and $R/l_0 \sim$ several 10). We therefore consider that the results obtained in the present work are applicable to aging phenomena observed within a time window of experiments on realistic spin glasses. However, mechanism which gives rise to the $\ln R$ dependence of $B_R$ is not clear yet. It might be related to fluctuations governed by the $T = T_c$ criticality since temperatures investigated in the present work may not be far enough from $T_c$. This problem is left for future work.
§4. Concluding Remarks

By means of Monte Carlo simulations we have studied aging dynamics after the temperature quench from $T = \infty$ to $T$ in the spin-glass phase in the 3D Ising EA model. The results of the energy evolution $e_T(t)$, in particular, the finite-size scaling on $\delta e_T(t) = e_T(t) - e_T(\infty)$, strongly suggest that the droplet picture describes aging dynamics appropriately. It is emphasized that these results are obtained based on eq. (1.1) which is a most fundamental ingredient of the droplet picture, and that they are extracted by analyzing time evolution of one spin configuration as compared with the previous works which were making use of the replica-overlap.

Also by analyzing relaxation times $\tau_L$ required for a global flip of spin configurations in small systems (isolated droplets) of size $L$, we have shown that the $L$-dependence of $\tau_L$ is consistent with the $t$-dependence of the mean domain size $R(t)$, i.e., $R(t \sim \tau_L(T)) \sim L$. This result further supports the droplet picture that coarsening of domain walls is in fact driven by successive nucleation of thermally activated droplets. The explicit form of this $t (\tau)$-dependence of $R(t) (L)$, however, disagrees with the original droplet theory due to Fisher and Huse: the barrier free energy associated with ordered domains of length scale $L$ is proportional not algebraically as predicted by the their theory but logarithmically to $L$.

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