General Scaling Theory of Magnetization and Susceptibility Profiles for a Semi-Infinite System

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We study the critical behavior of the magnetization profile \(m(z)\) and the susceptibility profile \(\chi(z)\) for a semi-infinite system. The scaling property of the surface magnetization \(m_s\) and the surface susceptibility \(\chi_s\), which are the integrated quantities of \(m(z)\) and \(\chi(z)\) respectively, are calculated for general temperature and magnetic field within the mean-field theory. The Monte Carlo method is applied to the study of \(m_s\) and \(\chi_s\) for a three-dimensional Ising model.

§ 1. Introduction

In the many particle physics, the translational invariance simplifies the problem greatly. The existence of a surface brings about the breaking of the translational symmetry for the direction perpendicular to the surface, which will be taken as a \(z\) axis, and makes the treatment of the problem difficult. On the other hand, the surface produces a lot of interesting effects. The surface effects on critical phenomena, which are full of variety, have been studied extensively in recent years.\(^{1,2}\)

When a system has a surface, various physical quantities have the \(z\) dependence. An example is a magnetization profile \(m(z)\), which was theoretically studied by several authors.\(^{3-5}\) Recently the Monte Carlo simulation was applied to the detailed study of the magnetization profile.\(^{6-8}\) However, the theoretical treatment so far has been restricted to the case that the external magnetic field \(h\) is zero. As for the equation of state for the surface system, a general scaling theory was developed by Okabe and Ohno.\(^9\) They calculated the scaling function for the surface equation of state within the mean-field approximation. In order to understand the scaling property of the magnetization profile near the critical point, the argument under general magnetic field is desirable.

In this paper, first, we calculate the magnetization profile \(m(z)\) and the susceptibility profile \(\chi(z)\) for general temperature and magnetic field within the mean-field theory, and discuss their scaling properties. Second, we calculate the surface magnetization \(m_s\) and the surface susceptibility \(\chi_s\), which are integrated quantities of \(m(z)\) and \(\chi(z)\) respectively, and obtain their scaling functions. We also calculate the universal critical amplitude ratios among the critical amplitudes for \(m_s\) and \(\chi_s\). Third, we use the Monte Carlo method to calculate \(m_s\) and \(\chi_s\) for a three-dimensional Ising model. We re-examine the “puzzling” disagreement of the amplitude ratio between the theory\(^5\) and the earlier Monte Carlo simulation.\(^1\) We show that our new Monte Carlo data are consistent with the results of the \(\varepsilon\) expansion.\(^5\) In the surface critical phenomena, the property of the transition varies according to the magnitude of the surface

\[
\begin{align*}
 f(z) &\to f_s \\
 m(z) &\to m_s \\
 \chi(z) &\to \chi_s
\end{align*}
\]

Table I. Schematic diagram of the calculation procedure for \(m(z), \chi(z), m_s\) and \(\chi_s\).
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exchange interaction $J_s$,\textsuperscript{11} but we confine ourselves to the case of the ordinary transition, the transition that bulk and surface order simultaneously at bulk $T_e$, in this paper.

In Table I, we schematically show the procedure to calculate $m(z)$, $\chi(z)$, $m_s$ and $\chi_s$ from the free energy profile $f(z)$ and the surface free energy $f_s$. Strictly, they are related to each other as follows:*)

\begin{align*}
m(z) &= -\frac{\partial f(z)}{\partial h} , \quad (1.1) \\
\chi(z) &= \frac{\partial m(z)}{\partial h} , \quad (1.2) \\
f_s &= \int_0^\infty dz [f(z) - f_b] , \quad (1.3) \\
m_b &= \int_0^\infty dz [m(z) - m_b] = -\frac{\partial f_s}{\partial h} , \quad (1.4) \\
\chi_b &= \int_0^\infty dz [\chi(z) - \chi_b] = \frac{\partial m_b}{\partial h} , \quad (1.5)
\end{align*}

where $f_s$, $m_b$ and $\chi_b$ are the free energy, magnetization and susceptibility for the bulk system, respectively.

\section*{§ 2. Mean-field theory for $m(z)$ and $\chi(z)$}

We consider the semi-infinite $\phi^4$ model in the mean-field approximation. The free-energy functional of our concern is

\begin{equation}
f[\phi(z)] = \int_0^\infty dz \left[ \frac{1}{2} \left( \frac{d\phi}{dz} \right)^2 + \frac{1}{2} t \phi^2 + \frac{1}{4} u \phi^4 - h \phi \right] , \quad (2.1)
\end{equation}

where $t = (T - T_e)/T_e$. The magnetization profile $m(z)$ is determined by minimizing the free energy. The functional differentiation of Eq. (2.1) leads to

\begin{equation}
\frac{d^2 m(z)}{dz^2} = tm(z) + um_b^3(z) - h . \quad (2.2)
\end{equation}

Noting that the bulk magnetization $m_b$ is given by

\begin{equation}
tm_b + um_b^3 = h , \quad (2.3)
\end{equation}

we have

\begin{equation}
\frac{dm(z)}{dz} = -(m(z) - m_b) \sqrt{\frac{t}{2} (m(z) + m_b)^2 + \frac{h}{m_b}} . \quad (2.4)
\end{equation}

Let us solve Eq. (2.4) under the boundary condition

\begin{equation}
m(-\lambda) = 0 , \quad (2.5)
\end{equation}

where $\lambda$ is the extrapolation length and $\lambda > 0$ for the ordinary transition. The elementary integration yields

\textsuperscript{*} We follow Ref. 5) for the definition of $f_s$, $m_s$ and $\chi_s$. They are different from the respective quantities in Ref. 1) by a minus sign.
\[ \tilde{m}(\tilde{z}) = \frac{m(z)}{m_b} = 1 - \frac{2 + p}{2 + p \cosh \tilde{z} + q \sinh \tilde{z}}, \tag{2.6} \]

where
\[ p = 2(2 + x), \tag{2.7} \]
\[ q = \sqrt{2(3 + x)(3 + 2x)} \tag{2.8} \]
and
\[ \tilde{z} = (z + \lambda) / \xi. \tag{2.9} \]

In the scaling argument the thermodynamic state is characterized by the variable \( x \) defined by
\[ x = \frac{t}{(m_b/B)^{1/\beta}}, \tag{2.10} \]

where \( \beta \) and \( B \) are the critical exponent and amplitude for the bulk spontaneous magnetization. We should note that \( x \) takes a value between \(-1\) and \(+\infty\). The phase boundary \((t < 0, h = 0)\), the critical isotherm \((t = 0, h > 0)\) and the critical isochore \((t > 0, h = 0)\) are represented by \( x = -1 \), \( x = 0 \) and \( x = +\infty \), respectively. In the mean-field theory, we have
\[ x = \frac{t}{u m_b^\beta}. \tag{2.11} \]

The correlation length \( \xi \), which has been used for normalizing the distance in Eq. (2.9), is given by
\[ \xi = \frac{1}{\sqrt{u m_b} \sqrt{3 + x}}. \tag{2.12} \]

For the limiting cases, Eq. (2.6) becomes
\[ \tilde{m}(\tilde{z}) = \tanh \frac{\tilde{z}}{2}, \quad x = -1, \tag{2.13a} \]
\[ \tilde{m}(\tilde{z}) = 1 - \frac{6}{2 + 4 \cosh \tilde{z} + 3\sqrt{2} \sinh \tilde{z}}, \quad x = 0, \tag{2.13b} \]
\[ \tilde{m}(\tilde{z}) = 1 - e^{-\tilde{z}}, \quad x = +\infty. \tag{2.13c} \]

Equation (2.13a) is well known as the mean-field form of the magnetization profile for the phase boundary.\(^{3,4}\) Since there exists no magnetization for the critical isochore, Eq. (2.13c) is considered to be a limiting form. We graphically show \( m(z)/m_b \) in Fig. 1. We find that the function gradually varies with the variation of \( x \). For small \( \tilde{z} \), \( \tilde{m}(\tilde{z}) \) becomes
\[ \tilde{m}(\tilde{z}) = \frac{q}{2 + p} \tilde{z} \quad \text{for} \quad \tilde{z} \ll 1. \tag{2.14} \]
It is expected from the scaling argument that \( \tilde{m}(\tilde{z}) \propto \tilde{z}^{(\beta_1 - \beta)/\nu} \) for \( \tilde{z} \ll 1 \). Using the mean-field values, \( \beta = 1/2 \), \( \nu = 1/2 \) and \( \beta_1 = 1 \), we find that this relation is satisfied. The large \( z \) behavior is obtained as

\[
1 - \tilde{m}(\tilde{z}) = \frac{2(2 + \rho)}{\rho + q} e^{-\tilde{z}} \quad \text{for } \tilde{z} \gg 1.
\]

We should note that \( 1 - m(z)/m_b \propto e^{-(z + 1)\xi} \) with the \( x \)-dependent \( \xi \). This fact can be used for the estimate of \( \xi \).

Next examine the susceptibility profile \( \chi(z) \). It is easily calculated by using Eq. (1.2). The result is

\[
\tilde{\chi}(\tilde{z}) = \frac{\chi(z)}{\chi_b} = \frac{1}{2 + \rho \cosh \tilde{z} + q \sinh \tilde{z}} \left[ 2 + \rho \right.
\]

\[
- \left( \frac{4 - \rho}{2 + \rho \cosh \tilde{z} + q \sinh \tilde{z}} \right) \left[ 4(\cosh \tilde{z} - 1) + 3((2 + \rho)/q) \sinh \tilde{z} \right] + 6 \tilde{z} (q \cosh \tilde{z} + p \sinh \tilde{z}) \left] \right.
\]

\[
\left. \right/ 2 + \rho \cosh \tilde{z} + q \sinh \tilde{z} \right);
\]

where we have used

\[
\chi_b = \frac{1}{u m_b^2} \frac{1}{3 + x}.
\]

Here \( \rho \), \( q \) and \( \tilde{z} \) are given by Eqs. (2.7), (2.8) and (2.9) respectively. For \( x = -1 \) Eq. (2.16) reduces to

\[
\tilde{\chi}(\tilde{z}) = 1 - \frac{1}{(1 + e^{\tilde{z}})^2} \left( 4 - \frac{e^{\tilde{z}} - e^{-\tilde{z}}}{2} - 3 \tilde{z} e^{\tilde{z}} \right),
\]

which is consistent with Eq. (4.22) in Ref. 5). We plot \( \chi(z)/\chi_b \) for \( x = -1, 0 \) and \( +\infty \) in Fig. 2. We see that the susceptibility profile varies continuously with the change of \( x \).
§ 3. Mean-field theory for $m_s$ and $\chi_s$

In this section we discuss $m_s$ and $\chi_s$, which are integrated variables of $m(z)$ and $\chi(z)$. First we consider the surface free energy $f_s$, which was already obtained as \cite{10,11}:

\[
\frac{f_s}{\sqrt{\frac{u}{2}m_b^3}} = -\frac{1}{3} \left[ (2(3+x))^{3/2} - (3+2x)^{3/2} \right] + 2\sqrt{2(3+x)} - \sqrt{3+2x} + 2(1+x)\ln\frac{2+\sqrt{2(3+x)}}{1+\sqrt{3+2x}}. \tag{3·1}
\]

As far as the leading scaling properties are concerned, we can put $\lambda \to 0$ for the ordinary transition. Therefore, we have omitted the correction terms in Eq. (3·1). Following Eq. (1·4), we can obtain $m_s$ either by differentiating $f_s$, Eq. (3·1), or by integrating $m(z)$, Eq. (2·6). Then we have

\[
m_s = -\sqrt{\frac{2}{u}}\ln\frac{2+\sqrt{2(3+x)}}{1+\sqrt{3+2x}}. \tag{3·2}
\]

We plot $-m_s/(2/u)^{1/2}$ as a function of $t$ for $\sqrt{u}h = 0$, 0.03 and 0.12 in Fig. 3. Normalizing $m_s$ by $m_b\xi$, we have the universal scaling form as

\[
\bar{m}_s = \frac{m_s}{m_b\xi} = -\sqrt{2(3+x)}\ln\frac{2+\sqrt{2(3+x)}}{1+\sqrt{3+2x}}. \tag{3·3}
\]

This scaling function is plotted in Fig. 4.

Next consider the surface susceptibility $\chi_s$. Calculating $\chi_s$ by both methods shown in Table 1, we can confirm the result. We find

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Fig. 3. Temperature dependence of $-m_s/(2/u)^{1/2}$ for $\sqrt{u}h = 0$ (curve a), 0.03 (curve b) and 0.12 (curve c).

Fig. 4. Plot of scaling function $-m_s/(m_b\xi)$ (mean-field).
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Fig. 5. Temperature dependence of $\chi_s$ for $\sqrt{u} h=0$ (curve a), 0.03 (curve b) and 0.12 (curve c).

\[ \chi_s = -\frac{1}{u^{3/2}m_0^3} \left( 3 + x \right)^{3/2} \frac{6x}{\sqrt{3 + 2x [2\sqrt{3 + 2x} + \sqrt{2(3 + x)}]}} \]  

(3.4)

Figure 5 is a plot of the $t$ dependence of $\chi_s$ as a function of $h$. The values of $h$ are the same as in Fig. 3. We should note that $\chi_s < 0$ for $t > 0$ and $\chi_s > 0$ for $t < 0$. The scaling function for $\chi_s$ is obtained as

\[ \tilde{\chi}_s = \frac{\chi_s}{\chi_s(0)} = \frac{-6x}{\sqrt{3 + 2x [2\sqrt{3 + 2x} + \sqrt{2(3 + x)}]}} \]  

(3.5)

We plot this scaling function in Fig. 6.

Let us discuss several universal amplitude ratios. We define critical amplitudes as follows:

\begin{align*}
    m_s &= B_s(-t)^{\eta_s}, & (t < 0, h = 0) \\
    \chi_s &= \Gamma_s t^{-\eta_s}, & (t > 0, h = 0) \\
    &= \Gamma_s'(-t)^{-\eta_s}, & (t < 0, h = 0) \\
    \xi &= \xi_0 t^{-\nu}, & (t > 0, h = 0) \\
    &= \xi_0'(-t)^{-\nu}. & (t < 0, h = 0)
\end{align*}

(3.6)-(3.12)

The bulk amplitudes $B$, $\Gamma$ and $\Gamma'$ are defined in the same manner as $B_s$, $\Gamma_s$ and $\Gamma_s'$. Taking an appropriate limit of the scaling functions, we can easily calculate the following universal amplitude ratios:

\[ \Gamma_s / \Gamma_s' = -\frac{4\sqrt{2}}{3}, \]  

(3.9)

\[ B_s / (B\xi_0) = \bar{m}_s(x = -1) = -2 \ln 2, \]  

(3.10)

\[ \Gamma_s / (\Gamma\xi_0) = \bar{\chi}_s(x = +\infty) = -1, \]  

(3.11)

\[ \Gamma_s' / (\Gamma'\xi_0') = \bar{\chi}_s(x = -1) = -\frac{3}{2}. \]  

(3.12)
These amplitude ratios are consistent with those obtained by the direct calculation of the amplitudes. 5)

§ 4. Monte Carlo study of $m_s$ and $\chi_s$

In the previous sections we have calculated $m(z)$, $\chi(z)$, $m_s$ and $\chi_s$ theoretically within the mean-field approximation. As a problem of a real system, let us consider a three-dimensional Ising model. The Monte Carlo simulation of the three-dimensional Ising model with a free boundary condition for the $z$ axis and with periodic boundary conditions for otherwise has been successfully utilized for the study of the surface effects on critical phenomena. Not only the critical exponents and critical amplitudes$^{6,7}$ but the general equation of state for the surface-layer magnetization $m_s^8$ have been investigated. The properties of the magnetization profile for general $t$ and $h$ have been studied in detail, and the information on the bulk correlation length has been obtained.$^{6-8}$ Moreover, the dynamic critical relaxation has been studied.$^{12}$ In the present paper we focus our attention on the surface magnetization $m_s$ and the surface susceptibility $\chi_s$. The difference of the total magnetization (susceptibility) between the free boundary system and the full periodic boundary system yields $m_s$ ($\chi_s$). We deal with the simple cubic Ising model of sizes $32 \times 32 \times 32$ and $32 \times 32 \times 64$. For the detailed explanation of the Monte Carlo method and the model, refer to Refs. 7) and 8). We fix the surface exchange coupling $J_s$ as $0.5J$ in the present study because the leading critical singularities of $m_s$ and $\chi_s$ do not depend on $J_s$. 11) As for the value of $T_c$ we take $J/kT_c=0.221564$. 13

In Fig. 7, we plot the $t$ dependence of $-m_s$ for various $h$. In contrast to the mean-field result, Fig. 3, $-m_s$ diverges as $t \to -0$ for $h=0$. The log-log plot of $-m_s$ versus $-t$ for $h=0$ is given in Fig. 8. According to the scaling relation among critical exponents,$^{11}$ we have $\beta_s = \beta - \nu$. It should be noted that $\beta_s = 0$ in the mean-field theory. The straight line given in this figure has the predicted slope $\beta_s = -0.305$ with the bulk values $\beta = 0.325$ and $\nu = 0.630$. 14 We see that the scaling relation is really satisfied. Estimating the critical amplitude $B_s$, defined by Eq. (3·6), we have $B_s = -0.51 \pm 0.03$. In Fig. 9, we show the log-log plot of $-m_s$ versus $h$ for $t=0$. On the critical isotherm $(t=0, h > 0)$, the dependence

$$m_s = D_s^{-1/\nu} h^{-1/\theta_s}$$  (4·1)

is expected. For the definition of the critical amplitude $D_s$, we have followed the conventional way of the bulk problem. Since $m_s < 0$ in the present case, the sign of

![Fig. 7. Monte Carlo result of the temperature dependence of $-m_s$ as a function of $h$ for $J_s=0.5J$. Solid curves are given for guiding the eye.](https://example.com/fig7.png)
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Fig. 8. Log-log plot of the \( t \) dependence of \(-m_s\).
The straight line has the predicted slope using the bulk values \( \beta = 0.325 \) and \( \nu = 0.630 \).

Fig. 9. Log-log plot of the \( h \) dependence of \(-m_s\) at \( T = T_c \).
The straight line shows the predicted slope using the bulk values.

\( D_s^{-1/8s} \) is minus. We give the straight line with the predicted slope \( 1/\delta_s = (\beta - \nu)/(\beta s) = -0.195 \) in the figure. The estimate of \( D_s \) is \( D_s^{-1/8s} = -0.39 \pm 0.01 \). Next discuss the scaling property of \( m_s \) for general \( t \) and \( h \). We may consider the scaling plot of \( m_s / (m_s \xi) \) against the scaled variable \( x \), Eq. (2.10), as in Fig. 4. Since the correlation length \( \xi \) is a secondary information, we employ another direct scaling plot for \( m_s \). In Fig. 10, we plot \( h^{1/8s}/(D_s^{1/8s} m_s) \) versus \( x \). This type of plot is frequently made for the bulk equation of state, and also made for the equation of state for the layer magnetization \( m_l \).

We see from the figure that the data for various \( h \) are collapsed on a single curve. From Eq. (3.2), we find that the scaling function in the mean-field approximation is expressed as

\[
\frac{h^{1/8s}}{D_s^{-1/8s} m_s} = \frac{\ln(2+\sqrt{6}) - \ln(1+\sqrt{3})}{\ln(2+\sqrt{2(3+x)}) - \ln(1+\sqrt{3+2x})}
\] (4.2)

with \( 1/\delta_s = 0 \). The dotted curve in Fig. 10 denotes the mean-field result. We find that the Monte Carlo result deviates from the mean-field one. The data of our scaling plot diverge as \( x \to -1 \), which reflects the fact that \( 1/\delta_s < 0 \) for the three-dimensional Ising model.

Next consider the surface susceptibility \( \chi_s \). We plot the \( t \) dependence of \( \chi_s \) for various \( h \) in Fig. 11. The qualitative behavior is the same as the mean-field result, Fig. 5; in the case \( h = 0 \), \( \chi_s < 0 \) for \( t > 0 \) and \( \chi_s > 0 \) for \( t < 0 \). The log-log plot of \( |\chi_s| \) versus \( t \) for \( h = 0 \) is given in Fig. 12. The straight line with the slope \( \gamma_s = \gamma + \nu = 1.87 \) is also given in the figure. The estimates of the critical amplitudes are \( T_s = -0.29 \pm 0.08 \) and \( T_s' = 0.23 \pm 0.05 \).

One comment should be made here on the surface coupling \( J_s \). We have estimated the critical amplitudes from the data for \( J_s = 0.5J \). Although the leading singularities of \( m_s \) and \( \chi_s \) are considered to be independent of \( J_s \), is \( m_s \) and \( \chi_s \) weakly depend on \( J_s \) as a correction. Therefore, if we estimate the critical amplitudes with-
Fig. 11. Monte Carlo result of the temperature dependence of $\chi_s$ as a function of $h$. The same symbols as in Fig. 7 are used. Solid curves are given for guiding the eye.

Fig. 12. Log-log plot of the $t$ dependence of $|\chi_\theta|$ for the high-temperature side (a) and the low-temperature side (b). The straight lines have a slope using the bulk values.

out considering this correction on the basis of the data for different $J_s$, there may exist some deviations. To check this point, we have also performed simulations for $J_s = 0.25J$ and $0.75J$. For $m_s$, we have found the systematic dependence on $J_s$, which is attributed to the corrections to the leading singularity. But the dependence is so weak that the deviations of the estimated amplitudes $B_s$ and $D_s$ are within the statistical errors. We have also found for the surface susceptibility $\chi_s$ that the deviations of the amplitudes due to the choice of $J_s$ are small.

Let us discuss the universal combination of the critical amplitudes.\(^5,9\) We obtained some other critical amplitudes in the previous Monte Carlo study.\(^7\) Together with the previous results, we have

$$\frac{\Gamma_s}{\Gamma_s'} = -1.3 \pm 0.5, \quad (4.3)$$

$$\frac{(\Gamma_s \Gamma_{1,1})}{\Gamma_1} = 1.0 \pm 0.5, \quad (4.4)$$

$$R_{\chi s}^{1/8} = (\Gamma_s D_s B_s^{5/3 - 1})^{1/8} = 1.4 \pm 0.2, \quad (4.5)$$

where $\Gamma_1$ and $\Gamma_{1,1}$ are the critical amplitudes of the layer susceptibility $\chi_1$ and the local susceptibility $\chi_{1,1}$, respectively.

Since the estimate of the amplitude ratios has rather large errors, we do not make a detailed comparison with the theory. But we make a short comment on $\Gamma_s/\Gamma_s'$. Diehl, Gompper and Speth\(^9\) calculated $\Gamma_s/\Gamma_s'$ by means of the $\epsilon$ expansion and showed that the $O(\epsilon)$ correction to the mean-field result, Eq. (3.9), is small. Therefore, the theoretical prediction of the sign of the ratio is minus. They cited the Monte Carlo data of the three-dimensional Ising model by Landau,\(^10\) which gives this ratio with a plus sign, and
questioned this “puzzling” disagreement. See Fig. 1 of Ref. 5). But our new Monte Carlo simulation clearly shows that the sign of $\Gamma_s/\Gamma_{s'}$ is minus. Contrary to the discussion by Diehl, Gompper and Speth,\textsuperscript{5} we conclude that the $\varepsilon$ expansion is effective for $\Gamma_s/\Gamma_{s'}$.

§ 5. Summary and discussion

We have calculated the magnetization profile $m(z)$ and the susceptibility profile $\chi(z)$ for a semi-infinite system within the mean-field theory. The surface magnetization $m_s$ and the surface susceptibility $\chi_s$ have been calculated for general temperature and magnetic field. Simulating a three-dimensional Ising model with a surface, we have investigated the scaling property of $m_s$ and $\chi_s$. We have shown that the amplitude ratio $\Gamma_s/\Gamma_{s'}$ is consistent with the theoretical result.\textsuperscript{5}

We finally make a short remark on the experimental research. Recently, various spin-polarized techniques, such as the spin-polarized low energy electron diffraction,\textsuperscript{15,16} the spin-polarized positron,\textsuperscript{17} and the spin-polarized photo-emission,\textsuperscript{18} have been applied to the precise measurement of critical properties near a surface. The experimental study of the magnetization profile, $m(z)$, or the change of the total magnetization due to the existence of a surface, $m_s$, is highly needed.

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