MAGNETIC PROPERTIES
OF THE THREE DIMENSIONAL ISING MODEL
WITH INTERFACE SINGLE–ION ANISOTROPY

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I. Introduction

Over several years, some attention have been directed to the spin-1 Ising model. In particular, because of the fundamental interest in the multicritical phenomena of physical systems, spin-1 model with single-ion anisotropy [1, 2] has been already investigated in some detail using a number of methods, namely the mean-field approximation (MFA) [1, 2], effective field approximation (EFT) [3, 4], high-temperature series expansion (HTSE) [5], constant coupling approximation (CCA) [6], Monte-Carlo technique (MC) [7], and so on. All of these approximation methods suggest the existence of a tricritical point at which the system changes from the second-order phase transition to the first-order one.

The influence of single-ion anisotropy on magnetic properties at or near the surface in semi-infinite systems has been studied. Thus, some recent experiment show that there exists a very strong anisotropy field acting in the surface or at an interface [8]. Such a system can be fabricated by growing a few atomic layers epitaxially on a magnetic substrate. In fact, the temperature dependences of the Auger polarizations from the rare earths Gd and Tb on the transition metal surfaces Fe(100) and Ni(100) have been obtained very recently [9]. Theoretically, Kaneyoshi has studied the surface magnetic properties of a semi-infinite spin-${1 \over 2}$ simple cubic Ising system with a spin-1 (100) free surface, in order to investigate the effect of surface single-ion anisotropy [10-12].

In this work we consider a simple cubic spin-${1 \over 2}$ Ising system which is divided, in two sides, by a spin-1 interface. The spin-1 atoms have a single-ion anisotropy. Thus, we investigate the effects of interface single-ion anisotropy on the interface coupled ferromagnetically to the two sides by the use of effective field theory (EFT) [13]. In particular we examine a new type of tricritical point at which the interface magnetization may change from second order to first order, depending on the strength of the perpendicular exchange with those in the next layers in the two sides. We also examine the effects of spin-1 interface coupled antiferromagnetically, to the two sides, on the interface magnetic property.

The outline of this paper is as follows: In section 2 we present the basic points of the theory. In section 3 we examine the phase diagrams and we give the reduced...
magnetization curves of interface and bulk for the ferromagnetic perpendicular exchange interaction case. The antiferromagnetic perpendicular exchange interaction case is given in section 4. Section 5 contains our conclusions.

2. The effective field theory

We consider a simple-cubic spin - $\frac{1}{2}$ Ising system with a spin -1 interface (fig. 1). The hamiltonian of the system is given by:

$$H = -J_0 \sum_{<i,j>} S_i S_j - J_1 \sum_{<i,m>} \mu_{im} \cdot S_i \cdot D_{nj} \sum_{<j,i>} (S_j)^2,$$  

where the summations are carried out only over nearest-neighbor pairs of spins. $S_i$ takes the values $\pm 1$ and $\mu_{im}$ can be $\pm 1$. $J_0$ is the exchange interaction in the two sides in the left and right of the interface. $J_1$ is the exchange interaction in the interface whereas $J_{2ij}$ is the perpendicular exchange parameter between spins at the interface and its nearest-neighbour spin $- \frac{1}{2}$ in the first layer in the left and in the right side of the interface. $D_{nj}$ is the single-ion anisotropy parameter at the interface.

The problem is now the evaluation of the mean values of $<S_i>$, $<(S_i)^2>$ and $<\mu_{im}>$. Using the differential operator technique [14] and introducing the following decoupling:

$$<S_i(S_i)^2>-<S_i>-<(S_i)^2>-<\mu_{im}>,$$

$$<\mu_{im}>-<\mu_{im}>.$$  

with $i \neq j$, $i = m$ and $m = n$, and $m = n$, $i = <\mu_{im}>$, the interface magnetization for the spin -1 interface can be defined as

$$m_1 = <S_0> = \left[ J_0 \cosh(V_{10}) + m_0 \sinh(V_{10}) + 1 - q_1 \right] x,$$

$$\left[ \cosh(V_{1}) + m_1 \sinh(V_{1}) \right] F_s(x) \left|_{x=0} \right.$$  

with

$$q_1 = <(S_0)^2>$$  

where $V = \frac{\partial}{\partial x}$ is a differential operator and $\beta = \frac{1}{k_B T}$. The angular bracket indicates the usual ensemble average.

$$<...> = \frac{\text{Tr} \left[ \exp \left(-\beta H \right) \right]}{\text{Tr} \left[ \exp \left(-\beta H \right) \right]}$$

The function $F_s(x)$ is defined by

$$F_s(x) = \frac{2 \cosh (\beta x)}{2 \cosh (\beta x) + \exp (-\beta D_s)}$$

In order to obtain $m_x$, it is also necessary to calculate the parameter $q_0$. In the same way as for the evaluation of $m_x$, we can easily obtain:

$$q_0 = \left[ J_0 \cosh(V_{10}) + m_0 \sinh(V_{10}) + 1 - q_1 \right] x,$$

$$\left[ \cosh(V_{1}) + m_1 \sinh(V_{1}) \right] F_s(x) \left|_{x=0} \right.$$  

with

$$G_s(x) = \frac{2 \cosh (\beta x)}{2 \cosh (\beta x) + \exp (-\beta D_s)}$$

The magnetization $\sigma_1$ of the first layer of side 1 (or side 2) is given by:

$$\sigma_1 = <\sigma_{i=1}> = \left[ \cosh(V_{1}) + \sigma_1 \sinh(V_{1}) \right] x,$$

$$\left[ \cosh(V_{1}) + \sigma_1 \sinh(V_{1}) \right] F_s(x) \left|_{x=0} \right.$$  

for the $n$th layer ($n \geq 2$) in side 1 (or side 2) we have

$$\sigma_n = \left[ \cosh(V_{1}) + \sigma_n \sinh(V_{1}) \right] x,$$

$$\left[ \cosh(V_{1}) + \sigma_n \sinh(V_{1}) \right] F_s(x) \left|_{x=0} \right.$$  

where $\sigma_{n-1}$ and $\sigma_{n+1}$ are the magnetizations in the $(n-1)$th and $(n+1)$th layers, respectively. In our present treatment, the bulk magnetization is given by putting $\sigma_n = \sigma_{n-1} = \sigma_{n+1} = \sigma_0$ into eq. (10).
3. Ferromagnetic perpendicular exchange interaction ($J_1 > 0$)

In this section we investigate the phase diagrams and the magnetization curves in the case where the interface is coupled ferromagnetically ($J_1 > 0$) to the two sides.

A. Phase diagrams

In order to examine the surface phase diagrams, we expand the right-hand sides of (2), (6), (8), (10) and (11), we obtained the polynomial equations of $m_x$, $q_x$, $\sigma_x$, $q_y$ and $\sigma_y$. According to refs [15, 16], let us assume that $\sigma_{n+1} = \sigma_n$ for $n > 1$, e.g., the magnetization of each layer with $n$ larger than $n = 1$ decreases exponentially into the bulk. Thus, the parameter $\gamma$ is given by, upon using the linearizing terms in eq (10),

$$\gamma = \frac{4C_1 - 2C_1 q_x^2}{2 - q_x^2}. \quad (12)$$

Also, linearizing eq (17) we can have

$$\sigma_x = \lambda_x m_x, \quad (13)$$

with

$$\lambda_x = \frac{B_1^0}{1 - 4B_1^0 + \gamma B_2^0}. \quad (14)$$

In the vicinity of the second-order phase transition line, the surface magnetization can be written as

$$m_s^2 = \frac{1}{\beta} a m_b \quad (15)$$

where the parameters $a$ and $b$ are given by

$$a = 4\lambda_1^0 + 2\lambda_2^0 \lambda_3. \quad (16)$$

The coefficients $C_1$, $B_1^0$, $B_2^0$, ... are given in the appendix.

In fig 2, by solving the equations ($a = 1$ and $b = 0$) numerically, the typical phase diagram of the present system is obtained where $\gamma J_1 > 0$ and the value of $a = \frac{1}{\gamma J_1}$ is changed. We denote the paramagnetic, bulk-ferromagnetic and interface-ferromagnetic phases by P, BF and IF, respectively. As seen from fig 2, the IF phase becomes wider more and more when the value of $a$ increases. Moreover, the critical value $\lambda_1$ of $\lambda$ vanishes for $\gamma = 1.888$. In the case $\gamma = 0$, which corresponds to two dimensional spin -1 Ising model, the critical temperature $T_c$ is given by $2.188$ compared with that obtained from MFA (2.688), HTSE (1.688) and mean field renormalization group (2.128) [17].

Fig. 3a shows the phase diagram in $[T, J_1, \gamma J_1]$ space which is exhibiting the surface tricritical behavior where $\Delta = 3.5$ and the value of $\alpha$ is selected. This tricritical behavior is obtained in the temperature region above the bulk transition temperature for the system. We note that the surface tricritical temperature increase with $\alpha$. In fig 3b, we found analogous surface tricritical behavior when the value of $\alpha$ is fixed ($\alpha = 3$) and the value of $\gamma$ is changed.

B. Magnetization curves

In order to obtain the thermal behaviors of the interface and layer magnetizations, it is necessary to solve the coupled equations (2), (6), (8) and (10). For this purpose, we expand the right-hand sides of eqs. (2), (6), (8) and (10), which gives

$$m_s^2 = 4\lambda_1^0 m_b + 2\lambda_2^0 \sigma_1 + 4\lambda_3^0 m_3 + 3\lambda_4 \sigma_1^2 m_b + 4\lambda_5^0 m_b \sigma_1^2 + 2\lambda_4 \sigma_1^3 + 4\lambda_5^3 \sigma_1^2 \quad (17)$$

The coefficients $C_1$, $B_1^0$, $B_2^0$, ... are given in the appendix.

In fig 2, by solving the equations ($a = 1$ and $b = 0$) numerically, the typical phase diagram of the present system is obtained where $\gamma J_1 > 0$ and the value of $a = \frac{1}{\gamma J_1}$ is changed. We denote the paramagnetic, bulk-ferromagnetic and interface-ferromagnetic phases by P, BF and IF, respectively. As seen from fig 2, the IF phase becomes wider more and more when the value of $a$ increases. Moreover, the critical value $\lambda_1$ of $\lambda$ vanishes for $\gamma = 1.888$. In the case $\gamma = 0$, which corresponds to two dimensional spin -1 Ising model, the critical temperature $T_c$ is given by $2.188$ compared with that obtained from MFA (2.688), HTSE (1.688) and mean field renormalization group (2.128) [17].

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\[ \sigma_i = 4B_i \sigma_i + B_j \sigma_j + B_k \sigma_k + 4B_4 \sigma_4 + B_5 \sigma_5 + B_6 \sigma_6 + 6B_\sigma \sigma_\sigma + 6B_\gamma \sigma_\gamma + m_k \]

\[ \sigma_\sigma = C_1 (\sigma_n + 4 \sigma_n + \sigma_{n+1}) + C_2 (4 \sigma_n + 6 \sigma_n + 4 \sigma_{n+1} + 4 \sigma_{n+1} - \sigma_n - \sigma_{n+1}) \]

\[ \phi = L_1 + \frac{1}{2} \sigma_1 m_k + \frac{1}{2} \sigma_2 m_k + L_2 \sigma_2 + 6L_4 \sigma_4 m_k^2 + L_5 m_k \]

where the coefficients \( A_i, B_i, C_i \) and \( L_i \) are given in the appendix. On the other hand, as \( n \to \infty \), \( \sigma_n \) should approach a bulk value \( \sigma_B \) determined from eq (11). However, the simplest method for solving eqs (19) - (21) is to assume that the magnetization remains unaltered after the third layer, namely, \( \sigma_4 = \sigma_5 = \ldots = \sigma_B \), which may be called the four-layer approximation. This approximation gives rather reasonable results for the thermal behavior of magnetization [13, 18, 79]. In figs (4a) and (4b) the temperature dependence of \( m_k \) and \( M \) is depicted by solving the eqs. (18) - (21). Note that the value of \( M \) is defined by:

\[ M = \frac{1}{2} \sigma_1 + 2 \sigma_2 + 2 \sigma_B \]  

In both figures the values of \( \sigma \) and \( \Delta \) are fixed as \( \sigma = 3 \) and \( \Delta = 3.5 \). Thus, in fig 3a the interface layer has a bulk transition temperature \( T_c^b = 3.75 \) whereas, in fig. 3b, the interface ordering temperature is in the temperature region higher than the bulk one. The same situation is also seen in the behavior of \( M \). Furthermore, in fig 4b, the \( m_k \) curve exhibits a small dip at \( T_c^b \). It indicates that the first derivative of \( m_k \) at \( T_c^b \) may have a discontinuity. Such a discontinuity is discussed in some experimental [20] and theoretical works [19, 21, 22, 23] in which the authors found no evidence for such discontinuity. As is discussed in ref [19, 22], our results show that the derivative of the interface magnetization at \( T_c^b \) depends strongly on the boundary conditions imposed in the calculation. This discontinuity is more apparent in \( \sigma_1 \) and \( \sigma_2 \) and consequently in \( M \) than in \( m_k \). Also shown in these figures are the results for the temperature dependence of the quadrupolar moment obtained as described in section 2. Furthermore, as is predicted in fig 3b, the transitions of \( m_k \) and \( M \) in fig (4a) and (4b) are of the second order.

The changes of interface magnetization \( m_k \) with \( T \) are depicted for selected values of \( \sigma \) in fig (5a) and (5b) for fixed values of \( \Delta = 4 \) and \( \Delta = 5.5 \) and \( D_s / J = -12.95 \), respectively. In these figures, if we put \( \sigma = 0 \), the system reduces to two-dimensional Blume-Capel model. Thus the interface magnetization shows the first order transition at \( T_c^f = 3.75 \) and \( T_c^b = 4.65 \) in figs (5a) and (5b), respectively. Furthermore, by increasing the value of \( \sigma \), in fig 5a, the gap width at the point where the interface magnetization changes discontinuously becomes smaller and finally reduces to zero. We find then a new type of tricritical behavior of the interface magnetization which depends on the strength of perpendicular exchange interaction \( J \). This tricritical behavior disappears after the vanishing gap and \( m_k \) changes to the continuous transition. The second order transition temperature is then given by the bulk transition temperature \( T_c^b \). On the other hand, in fig 5b, the discontinuity of \( m_k \) is shown at temperatures lower and higher than \( T_c^b \). Then the second order transition temperature of the system occurs at \( T_c^b > T_c^f \). Tricritical behavior of \( m_k \) is also obtained and depends on the value of \( D_s / J \). In fig 6, the interface magnetization is depicted for the system with \( \sigma = 5 \) and \( \Delta = 3.5 \) by changing the value of \( D_s / J \). The first order transition temperature for \( m_k \) is given at \( T_c^f < T_c^b \).

IV. Antiferromagnetic perpendicular exchange interaction \( (J_1 < 0) \)

In this case the interface layer is coupled antiferromagnetically to the two bulk-sides \( (J_1 < 0) \). Experimentally, in the semi-infinite systems, Gd couples antiferromagnetically to both Fe and Ni and Tb exhibits antiferromagnetic coupling to Fe if deposited in the submonolayer range. In these systems, the magnitude of the spins on the surface is clearly different from that in the bulk.
Fig 7a shows the numerical results when the values of $D_S$ and $J_B$ are fixed as $D_S^B = 0$ and $A = 0$. In the figure, the temperature dependences of $\langle m_s \rangle$ is depicted when the values of $\alpha$ is changed as $\alpha = -1$, $-0.5$, and $-0.1$. Also, the thermal variation of $\phi$ is also plotted. Thus, a linear temperature dependence of $\langle m_s \rangle$ has been observed in the case $\alpha = -1$. For $1 > \alpha > 0$, the surface magnetization $\langle m_s \rangle$ exhibits a weak downward curvature. This behavior of $\langle m_s \rangle$ is shown in some theoretical [12] and experimental works [21]. Experimentally, the temperature dependence of the Auger-electron spin-polarization of the resonant $N_{13}N_{13}N_{13}$ emission of two Gd films on Ni (100) express the weak downward curvature for the thermal variation.

In fig. 7b, the magnetization curves $\langle m_s \rangle$ and $M$ are investigated for the system with $A = 1.5$ and $D_S^B = 0$, for different values of $\alpha$. For $\alpha = 1$, the behavior of $M$ is analogous as that obtained in the ferromagnetic case ($\alpha > 0$). For $1 > \alpha > 0$, a finite magnetization of $M$ is obtained in the temperature region $T^b_c < T < T^b_c$ where $T^b_c$ is the surface ordering temperature. In order to clarify the behavior of $M$ in the vicinity of $T^b_c$, the insert expresses the thermal variations, for $\alpha = 1$, of $M$ and $\langle m_s \rangle$ by taking a larger scale, which clearly shows that the compensation point $T = T^{comp}$ is obtained at a temperature a little smaller than the bulk $T^{b}_c$. A similar phenomenon ($T^{comp} < T^{b}_c$) is found in recent experiments for Gd and Tb films on W [24, 25], for which the surface magnetization is coupled antiferromagnetically to the bulk.

V. Conclusion

We have discussed the effects of interface single-ion anisotropic and perpendicular exchange interaction ($J_1$) on the transition temperature for interface ordering, interface tricritical point, and phase diagrams within the framework of effective field theory and the four layer approximation. The interface magnetization should exhibit a first order transition at the transition temperature $T^b_c$ or $T^b_c$, when we take appropriate values $\alpha$, $D_S$, $A$ and $J_1$ ($J > 0$) in figs. 3. Furthermore, as shown in figs 5, we find a new type of tricritical behavior of interface magnetization depending on the strength of the perpendicular exchange interaction $J_1$. This behavior appears at $T < T^b_c$ (fig 5a) and $T > T^b_c$ (fig 5b).

Finally, for $J_1 < 0$, the interface magnetization $\langle m_s \rangle$ exhibits a weak downward curvature for $J_1 < J$ (fig 7a). In fig 7b, the interface orders at $T^b_c > T^b_c$ and we obtain a finite magnetization of $\langle m_s \rangle$ in the temperature region $T^b_c < T < T^b_c$. Before $T^b_c$ a compensation point $T^{comp}$ is obtained. These two phenomena are found in several experimental works.

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Appendix

\[ A_1 = [q_0 (\cosh(V_J^2) - 1) + 1] \sinh(V_J) \cosh^2(V_J) \mathcal{F}_S(x) \bigg|_{x=0} \]
\[ A_2 = [q_0 (\cosh(V_J^2) - 1) + 1] \sinh(V_J) \cosh(V_J) \mathcal{F}_S(x) \bigg|_{x=0} \]
\[ A_3 = [q_0 (\cosh(V_J^2) - 1) + 1] \sinh(V_J) \cosh(V_J) \mathcal{F}_S(x) \bigg|_{x=0} \]
\[ A_4 = [q_0 (\cosh(V_J^2) - 1) + 1] \sinh^2(V_J) \sinh(V_J) \cosh(V_J) \mathcal{F}_S(x) \bigg|_{x=0} \]
\[ A_5 = [q_0 (\cosh(V_J^2) - 1) + 1] \sinh^2(V_J) \cosh(V_J) \mathcal{F}_S(x) \bigg|_{x=0} \]
\[ A_6 = \sinh^4(V_J) \sinh(V_J) \cosh(V_J) \mathcal{F}_S(x) \bigg|_{x=0} \]
\[ A_7 = [q_0 (\cosh(V_J^2) - 1) + 1] \sinh^4(V_J) \cosh(V_J) \mathcal{F}_S(x) \bigg|_{x=0} \]
\[ B_1 = [q_0 (\cosh(V_J^2) - 1) + 1] \sinh(V_J) \cosh(V_J) \mathcal{F}_S(x) \bigg|_{x=0} \]
\[ B_2 = [q_0 (\cosh(V_J^2) - 1) + 1] \sinh^2(V_J) \cosh(V_J) \mathcal{F}_S(x) \bigg|_{x=0} \]
\[ B_3 = \cosh^2(V_J) \sinh(V_J) \mathcal{F}_S(x) \bigg|_{x=0} \]
\[ B_4 = [q_0 (\cosh(V_J^2) - 1) + 1] \sinh^2(V_J) \mathcal{F}_S(x) \bigg|_{x=0} \]
\[ B_5 = \sinh^4(V_J) \cosh(V_J) \sinh(V_J) \mathcal{F}_S(x) \bigg|_{x=0} \]

The coefficients \( A_1^0, B_1^0, q_0, q_1 \) and \( A_2^0 \) are given by:

\[ A_1^0 = A_1 \text{ (in which } q_0 \text{ is replaced by } q_0) \]
\[ B_1^0 = B_1 \text{ (in which } q_0 \text{ is replaced by } q_0) \]
\[ A_1^0 = [q_0 (\cosh(V_J^2) - 1) + 1] \sinh^2(V_J) \cosh^2(V_J) \mathcal{F}_S(x) \bigg|_{x=0} \]
\[ A_2^0 = [q_0 (\cosh(V_J^2) - 1) + 1] \sinh^2(V_J) \cosh(V_J) \mathcal{F}_S(x) \bigg|_{x=0} \]

The parameters \( \theta_3 \) and \( \theta_4 \) are obtained by substituting \( q_0 \) as:

\[ \theta_3 = \theta_4 = \frac{1}{2} \]

Here, \( \theta_3 \) and \( \theta_4 \) are defined by:

\[ \theta_3 = \frac{1}{2} \]

\[ \theta_4 = \frac{1}{2} \]

where

\[ \theta_3^0 = \theta_3 \text{ (by replacing } q_0 \text{ by } q_0) \]

\[ \theta_4^0 = \theta_4 \text{ (by replacing } q_0 \text{ by } q_0) \]

\[ L_4 = [q_0 (\cosh(V_J^2) - 1) + 1] \sinh^2(V_J) \cosh^2(V_J) \mathcal{F}_S(x) \bigg|_{x=0} \]
References

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Figure captions

Fig. 1: Part of a two-dimensional cross section through an infinite Ising lattice with an interface single-ion anisotropy. Black points denote the lattice positions, in two sides (1) and (2), which are occupied by spins $a_1 = 1$. On the interface, the lattice points are occupied by $S_j = \pm 1$ and 0.

Fig. 2: Phase diagram in the $(T, \Delta)$ space of the system with $D_N/T = 0$ and selected values of $\alpha$. The paramagnetic, bulk-ferromagnetic and interface-ferromagnetic phases are indicated by P, BF and IF, respectively.

Fig. 3: Surface transition temperatures of the system in $(T, \Delta)$ plane with $\Delta = 3.5$ and selected values of $\alpha$ (fig 3a) and $\alpha = 5$ when the value of $\Delta$ is changed (fig 3b). The black points denote the transition points and the dashed lines express the first order phase transition.

Fig. 4: The temperature dependence of $m_s, M$ and $\theta$, for the system with $\alpha = 5$ and $\Delta = 3.5$ when the value of $q_1$ is given as $D_N/T = 0$ (fig 4a) or $D_N/T = \pm 5$ (fig 4b). The dashed line in fig 4b is for reduced magnetization curve of bulk $\theta_B$.

Fig. 5: Temperature dependence of $m_s$ for the system with $\Delta = 3.5$, $D_N/T = -9.8$ when the value of $\Delta$ is changed as follows: $a: \alpha = 0$, $b: \alpha = 1$, $c: \alpha = 2$, $d: \alpha = 3$, $e: \alpha = 5$ (fig 5a) and $D_N/T = -12.05$ and $\alpha$ takes the values $a: \alpha = 0$, $b: \alpha = 1$, $c: \alpha = 5$, $d: \alpha = 1$, $e: \alpha = 1.5$, $f: \alpha = 1.7$ (fig 5b).

Fig. 6: Thermal behavior of $m_s$ with $\alpha = 5$ and $\Delta = 3.5$ when the value of $D_N/T$ is selected as $a: D_N/T = -10$, $b: D_N/T = -9.6$, $c: D_N/T = -9.34$, and $d: D_N/T = -8.6$.

Fig. 7: Temperature dependence of $m_s$ for the system with $D_N = 0$ when the value of $\alpha$ is given by $\alpha = -1$, $-5$ and $-1$ (fig 7a). In fig 7b, the thermal behavior of $m_s$ and $M$ for $D_N = 0$, $\Delta = 1.5$ and several values of $\alpha$. The insert is the temperature dependence of $M$ and $\theta_B$ in the vicinity of $T = \theta_B^0$. 

13

14
Fig. 7b

\[ \Delta = 1.5 \]

\[ \frac{D}{J} = 0 \]

\[ \alpha = -1 \text{, } -0.5 \text{, } -0.1 \]

\[ m_0 \]

\[ M \]

\[ t_c^B \]

\[ t_c \]

\[ \tau_{comp} \]

\[ |M| \]