

Wetting and layering transitions of a spin-1/2 Ising model in a random transverse field method

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The effect of a random transverse field (RTF) on the wetting and layering transitions of a spin-1/2 Ising model, in the presence of bulk and surface fields, is studied within an effective field theory by using the differential operator technique. Indeed, the dependencies of the wetting temperature and wetting transverse field on the probability of the presence of a transverse field are established. For specific values of the surface field we show the existence of a critical probability p_c above which wetting and layering transitions disappear.

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I. INTRODUCTION

Recently much attention has been directed to study the wetting and layering transitions of magnetic surfaces Ising model. Experimental studies have motivated much theoretical works in order to understand and explain the growth of thin layers from only single atoms. A simple lattice-gas model with layering transitions has been introduced and studied in the mean field approximation by de Oliveira and Griffiths [1]. Multilayer films adsorbed on attractive substrates may exhibit a variety of possible phase transitions, as has been reviewed by Pandit *et al.* [2], Nightingale *et al.* [3], Patrykiewicz *et al.* [4] and Ebner *et al.* [5-8]. One type of transitions is the layering transitions, in which the thickness of a solid film increases discontinuously by one layer as the pressure is increased. Such transitions have been observed in a variety of systems including for example ⁴He [9,10] and ethylene [11,12] adsorbed on graphite. Ebner and Saam [13] carried out Monte Carlo simulations of such a lattice gas model. Huse [14] applied renormalization group technique to this model. It allowed the study of the effects on an atomic scale in the adsorbed layers. The lattice gas models applied to the wetting phenomena was reviewed by Dietrich [15]. The effect of finite size on such transitions has been studied, in a thin film confined between parallel planes or walls, by Nakanishi and Fisher [16] using mean field theory.

The model of transverse field was originally introduced by de Gennes [17] for hydrogen-bonded ferroelectrics such as KH₂PO₄. Since then, this model has been applied to several physical systems, like DyVO₂, and studied by a variety of sophisticated techniques [18-21]. The technique of differential operator introduced by Kaneyoshi [22] is as simple as the mean field method and uses a generalised but

approximate Callen relation derived by Sa Barreto and Fittipaldi [23]. The system has a finite transition temperature, which can be decreased by increasing the transverse field to a critical value Ω_c . The effect of a transverse field on the critical behaviour and the magnetisation curves was studied [18-21] and by Kaneyoshi *et al.* [24,25]. Using the perturbative theory, Harris *et al.* [26] have studied the layering transitions at $T=0$ in the presence of a transverse field. Benyoussef and Ez-Zahraouy have studied the layering transitions of Ising model thin films using a real space renormalization group [27], and transfer matrix [28] methods.

On the other hand, the random systems have been known to be dominated by rare regions. This effect is particularly pronounced for random quantum systems at low or zero temperature far from critical points. Indeed, Griffiths [29] showed that the free energy is a non analytic function, because of rare regions. Having found all the derivatives being finite, Harris [30] concluded that this effect was very weak for classical systems.

The simplest of all random quantum systems is the random transverse Ising model [31,32] (and references therein). Using the mean field theory, we have studied in a previous work [33], the wetting and layering transitions of a spin-1/2 Ising model in the presence of a uniform transverse field.

Our aim in this work is to study the effect of a random transverse field (RTF), on the wetting and layering transitions of a spin-1/2 Ising system, within an effective field theory (EFT) by using the differential operator technique.

The outline of this paper is as follows. In Section 2 we present the formalism and the method. In Section 3 we investigate and discuss the phase diagrams.

II. MODEL AND METHOD

Transverse and longitudinal magnetic fields are applied to a system with N coupled ferromagnetic layers. The Hamiltonian can be written as

$$H = - \sum_{\langle ij \rangle} J_{ij} S_i^z S_j^z - \sum_i (\Omega S_i^x + H_i S_i^z) \quad (1)$$

where the first summation is carried out only over nearest-neighbour pairs of spins, S_i^μ , ($\mu=x,z$) are the Pauli matrices of a spin-1/2 and $J_{ij}=J$ is the exchange interaction assumed to be constant. H_i is the longitudinal field applied on the site 'i', assumed to be uniform in a layer 'k', and defined by:

$$\begin{aligned} H_k &= H + H_{S1} \quad \text{for} \quad k=1 \\ &= H \quad \text{for} \quad 1 < k < N \\ &= H + H_{S2} \quad \text{for} \quad k=N \end{aligned} \quad (2)$$

where the surface fields H_{S1} and $H_{S2} = -H_{S1}$ are applied on the first layer $k=1$ and the last layer $k=N$, respectively. H is the longitudinal field. The transverse field Ω is governed by the probability distribution law:

$$P\{\Omega\} = p\delta(\Omega - \Omega_0) + (1-p)\delta(\Omega) \quad (3)$$

with $0 \leq p \leq 1$. The case $p=0$ corresponds to the absence of the transverse field, whereas $p=1$ is a situation with a uniform transverse field $\Omega = \Omega_0$.

We will use an effective field theory which neglects correlation between spins [35-36], but it takes into account the relations such as $\langle (s_i)^2 \rangle = 1$ exactly, where $\langle \dots \rangle$ denotes the thermal average. This method has been used by several authors to study quantum systems [18,22-25], and disordered systems [18,19,21,37,38]. It is based on a cluster comprising a single selected site labelled 'i' and the neighbouring sites with which it directly interacts.

Hence, the part of the Hamiltonian containing the site 'i', is given by

$$h_i = \left(\sum_{jj \neq i} J_{ij} S_j^z + H_i \right) S_i^z + \Omega S_i^x \quad (4)$$

the summation runs over nearest neighbour sites 'j' of the site 'i'. The diagonalization of the operator h_i leads

to the eigen values $\lambda_i^\pm = \pm \sqrt{x_i^2 + \Omega^2}$ with

$$x_i = \sum_{jj \neq i} J_{ij} S_j^z + H_i \quad \text{and} \quad J_{ij} = J.$$

In the next we will use the notation $\sigma_i^Z = 2S_i^Z$. Following Sa Barreto and Fittipaldi [23] we write the approximate relation:

$$\langle \sigma_i^z \rangle_c = \frac{\text{Tr}(\sigma_i^z \exp(-\beta h_i))}{\text{Tr}(\exp(-\beta h_i))} \quad (5)$$

where $\beta = 1/(k_B T)$, $\langle \dots \rangle_c$ indicates the mean value of σ_i^Z for a given configuration 'c' of all other spins, $\langle \dots \rangle$ denotes the average over all spin configurations.

Equations (5) are not exact for an Ising system with a transverse field, nevertheless, they have been accepted as a reasonable starting point in many studies [22,23]. After averaging over the probability distribution p , the longitudinal magnetisation of a layer k , is given by

$$m_k^z = p \langle f_\Omega(x_k) \rangle + (1-p) \langle f_0(x_k) \rangle \quad (6)$$

with the functions $f_\Omega(x)$ and $f_0(x)$ are defined, respectively, by

$$f_\Omega(x) = \frac{x}{\sqrt{x^2 + \Omega^2}} \tanh(\beta \sqrt{x^2 + \Omega^2}) \quad (7)$$

$$f_0(x) = \tanh(\beta x) \quad (8)$$

Introducing the differential operator defined by:

$$\exp(\alpha D) f_\mu(x) = f_\mu(x + \alpha), (\mu = \Omega, 0) \quad (9)$$

where $D = d/dx$, we can write the longitudinal magnetisation of a plane 'k' as :

$$\begin{aligned} m_k^z &= p [\exp(\langle x_k \rangle D)] f_\Omega(x_k) \Big|_{x=0}^p + \\ &+ (1-p) [\exp(\langle x_k \rangle D)] f_0(x_k) \Big|_{x=0}^p \end{aligned} \quad (10)$$

For a cubic lattice model, each site is in interaction with 6 neighbours, one can write the magnetisation as

$$\begin{aligned} m_k^z &= p [(\cosh JD + \langle \sigma_k^z \rangle \sinh JD)^4 \times \\ &(\cosh JD + \langle \sigma_{k-1}^z \rangle \sinh JD) \times \\ &(\cosh JD + \langle \sigma_{k+1}^z \rangle \sinh JD) \times \\ &(\exp(H_k D)) f_\Omega(x) \Big|_{x=0}^p] + (1-p) \times \\ &[(\cosh JD + \langle \sigma_k^z \rangle \sinh JD)^4 \times \\ &(\cosh JD + \langle \sigma_{k-1}^z \rangle \sinh JD) \times \\ &(\cosh JD + \langle \sigma_{k+1}^z \rangle \sinh JD) \times \\ &(\exp(H_k D)) f_0(x) \Big|_{x=0}^p] \end{aligned} \quad (11)$$

with the boundary conditions $m_{N+1}^Z = m_0^Z = 0$.

Neglecting the correlations, so that :

$$\langle \sigma_i^z \sigma_j^z \dots \sigma_l^z \rangle = \langle \sigma_i^z \rangle \langle \sigma_j^z \rangle \dots \langle \sigma_l^z \rangle \quad (12)$$

and using the differential operator, the final expression of the magnetisation is:

$$\begin{aligned} m_k^z = & B_0(p, \Omega) + B_1(p, \Omega) \langle \sigma_k^z \rangle + \\ & B_2(p, \Omega) \langle \sigma_k^z \rangle^2 + B_3(p, \Omega) \langle \sigma_k^z \rangle^3 + \\ & B_4(p, \Omega) \langle \sigma_k^z \rangle^4 + \dots + B_{19}(p, \Omega) \langle \sigma_k^z \rangle^{19} + \\ & B_{20}(p, \Omega) \langle \sigma_k^z \rangle^{20} \end{aligned} \quad (13)$$

where $B_l(p, \Omega) = pA_l(\Omega) + (1-p)A_l(0)$, $l=0,1,\dots,19$, and the coefficients $A_l(\mu)$, ($\mu=\Omega,0$), $l=0,1,\dots,19$; are given in the Appendix.

Similarly, the transverse magnetisation $\langle \sigma_k^x \rangle$, of a layer 'k', can be formulated using a function $g_\mu(x)$ instead of the function $f_\mu(x)$, but in this work, we are essentially interested in the wetting phenomena which is essentially governed by the longitudinal magnetisation $\langle \sigma_k^z \rangle$.

III. RESULTS AND DISCUSSION

In this section we present phase diagrams and longitudinal magnetisations of the model (1) described in section 2. The ground state of this model was established in a previous work [33].

In the following we limit our calculations to $N = 20$ layers. The results are found to be similar for an arbitrary larger number of layers $N > 20$. We will distinguish between two cases, namely:

- i) $p=1.0$: uniform transverse field,
- ii) $0 < p < 1$: random transverse field.

The start point is a situation where all the spins are down. For fixed values of H_{S1}/J and Ω/J , there exist a temperature T_w/J such that:

- i) for $T/J < T_w/J$ the spins of all layers are down for $H/J < 0$ and up once $H/J > 0$, with the coexistence of the two cases at $H/J=0$,

- ii) for $T/J > T_w/J$ and increasing the bulk field H/J

the spins of the first layer will flip and become up: this is the surface transition. Increasing the bulk field more and more, the spins of the second layer will flip up, and so on. For a sufficiently large number of layers N , the complete wetting is reached when the number of layering transitions is close to the number of layers at $H/J=0$. T_w/J is the wetting temperature. Similarly, the wetting transverse field Ω_w/J is obtained for fixed values of H_{S1}/J and T/J , and increasing the bulk field H/J .

Hereafter, the surface field effect on the parameters T_w/J and Ω_w/J will be discussed for $p=1$. The notation $1^k 0^{N-k}$ is a situation where k layers are spin-up while $N-k$ layers are spin-down from the top surface $k=1$ to the surface of the bottom $k=N$.

In order to study the behaviour of the system under the effect of the temperature, for fixed surface field H_{S1}/J and transverse field, we plot in Fig. 1 the corresponding phase diagrams: (a) in absence of transverse field $\Omega/J=0.0$ and (b) in the presence of a transverse field $\Omega/J=1.0$.

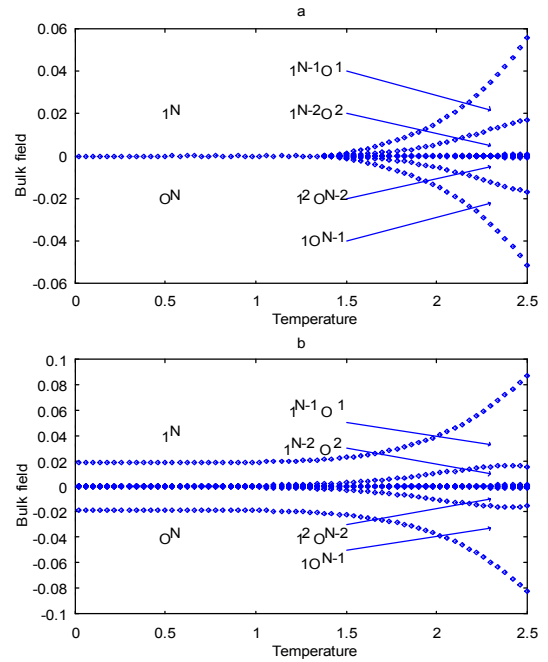


FIG. 1 : Phase diagram in the $(H/J, T/J)$ plane for a pure system ($p=1.0$) with the surface fields ($H_{S1}/J=0.998, H_{S2}/J=-H_{S1}/J$) :
a) $\Omega/J=0.0$, b) $\Omega/J=1.0$.

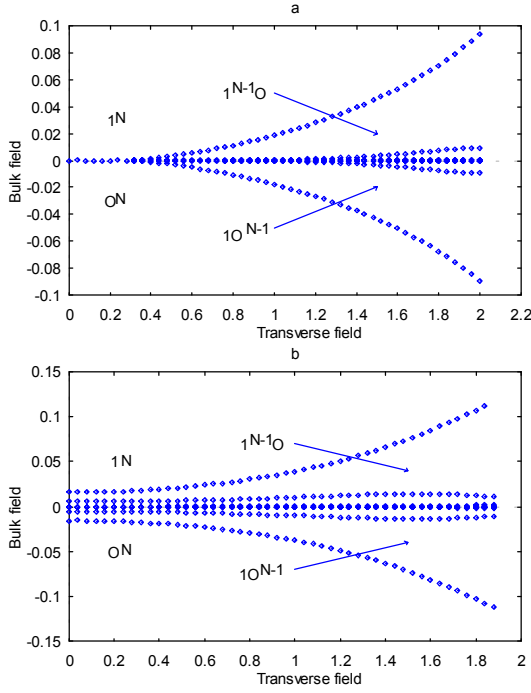


FIG. 2 : Phase diagram in the $(H/J, \Omega/J)$ plane for a pure system ($p=1.0$) with $(H_{S1}/J=0.998, H_{S2}/J=-H_{S1}/J)$, a) $T/J=0.5$, b) $T/J=2.0$.

One can note that the effect of increasing the transverse field is to decrease T_W/J .

When increasing the temperature the wetting transverse field Ω_W/J decreases. This is shown in Fig. 2(a) for a lower temperature $T/J=0.5$, and Fig. 2(b) for higher temperature $T/J=2.0$. We can note the absence, in Figs. 1(b) and 2(b), of the transitions: $ON \leftrightarrow 1N$. Indeed, these transitions subsist for $\Omega/J=0.0$ and lower temperature, Figs. 1(a) and 2(a) respectively, in agreement with the ground state [33].

Examining the magnetisation behaviour we found that it decreases rapidly in the transition zone either when increasing the temperature as it is shown in Fig. 3(a) for $\Omega/J=1.0$, or when increasing the transverse field as it is plotted in Fig. 3(b) for $T/J=0.02$. Positive magnetisations, in these figures, are calculated for a bulk field $H/J \rightarrow 0^+$, whereas the negative values correspond to $H/J \rightarrow 0^-$.

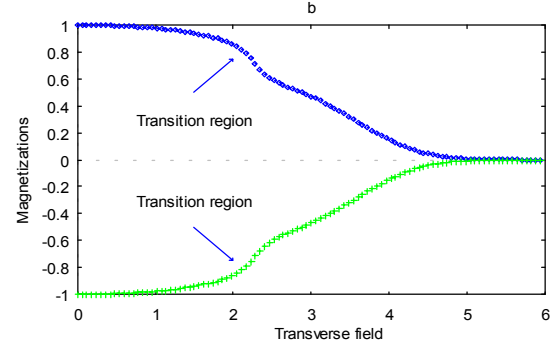
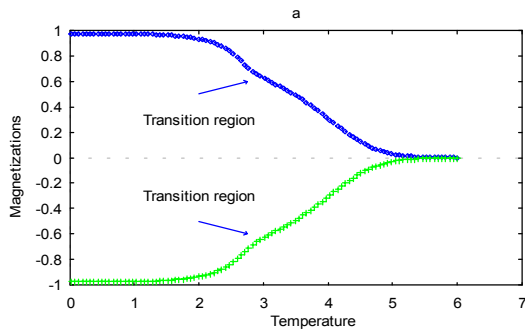


FIG. 3 : Magnetisations for $(H_{S1}/J=0.95, H_{S2}/J=-H_{S1}/J)$: a) as function of the temperature for $\Omega/J=1.0$, b) as function of the transverse field for $T/J=0.02$.

In order to study the effect of a random transverse field $0 < p < 1$ on the wetting and layering transitions, we introduce the probability law given in Eq. (3). The corresponding phase diagrams in the space $(T/J, \Omega/J, p)$, are plotted in Fig. 4, for $H_{S1}/J=0.95$. It is important to note here the existence of a critical value p_c , of the probability p , above which the wetting transitions disappears. The numerical value corresponding to Fig. 4 is $p_c = 0.0885$. This critical probability p_c depends on the surface field H_{S1}/J .

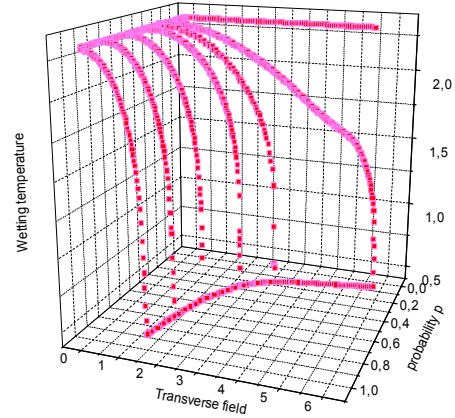


FIG. 4 : Phase diagrams in the $(T/J, \Omega/J, p)$ space for $(H_{S1}/J=0.95, H_{S2}/J=-H_{S1}/J)$.

As it is illustrated in Fig. 5, p_c decreases linearly for values of $H_{S1}/J < 0.85$, and almost linearly for $H_{S1}/J > 0.85$, with a discontinuity point for $H_{S1}/J = 0.85$. A similar result was found by Harris [34], for a disordered system with bond and site dilutions, showing that the critical transverse field at zero temperature presents a discontinuity as the concentration passes through the critical percolation concentration.

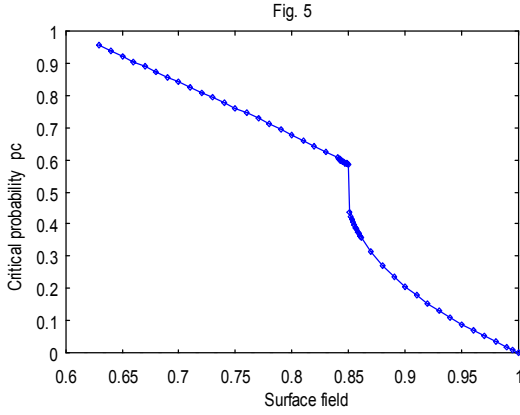


FIG. 5: The critical probability p_c dependence on the surface field H_{S1}/J for $T/J=0.02$.

Below, we will consider the effect of the surface field, and the probability p , on the wetting temperature T_w/J and the wetting transverse field Ω_w/J . Indeed, T_w/J vanishes as well as increasing the surface field at fixed probability value, Fig. 6(a), or increasing the probability at fixed surface field value, Fig. 6(b).

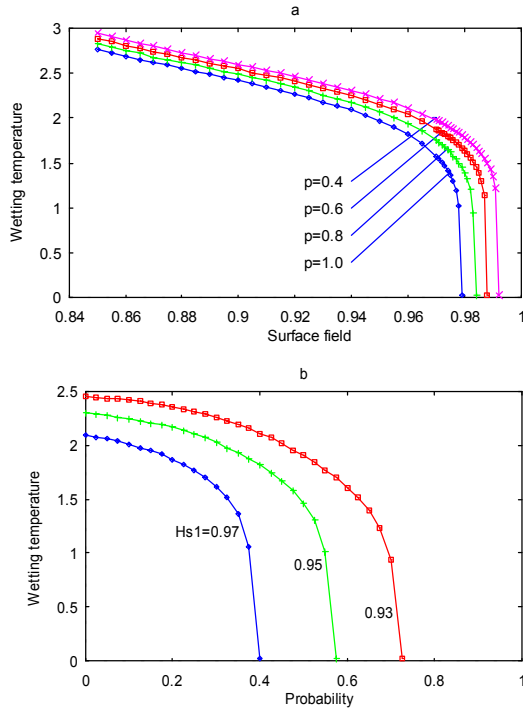


FIG. 6: Wetting temperature T_w/J as a function of: a) surface field H_{S1}/J for $\Omega/J=1.0$ and several values of the probability p ; b) probability p for $\Omega/J=2.0$ and several values of the surface field H_{S1}/J .

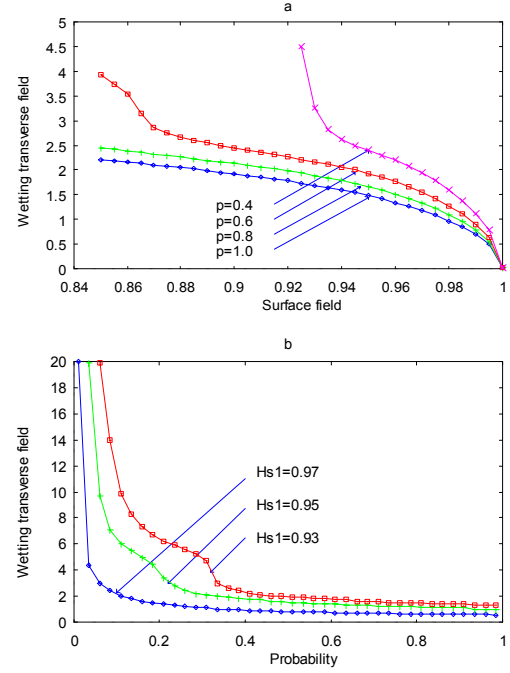


FIG. 7 : Wetting transverse field Ω_w/J as a function of : a) surface field H_{S1}/J for $T/J=0.02$ and several values of the probability p ; b) probability p for $T/J=2.0$ and several values of the surface field H_{S1}/J .

While Ω_w/J does not exhibit the same behaviour. However, it decreases when increasing the surface field for a fixed probability value p , Fig. 7(a). Whereas it diverges for a fixed surface field value for sufficiently small value of p as it is illustrated in Fig. 7(b). Furthermore, these figures show that the surface field value making $T_w/J=0$ increases for decreasing p , whereas the surface field value for which $\Omega_w/J=0$ is close to 1.

IV . CONCLUSION

Within the effective field theory (EFT) and using the differential operator technique, we have studied the phase diagrams of wetting and layering transitions of a spin-1/2 Ising model, for a random transverse field (RTF). It is found that, in the pure case $p=1$, this system exhibits the same behaviour as the mean field study [33]. The dependency of the wetting temperature and wetting transverse field on the surface field and the probability of the presence of a transverse field, was investigated.

We have showed the existence of a critical probability p_c above which the wetting and layering transitions disappear.

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Appendix A: Expression of the coefficients $A_k(\mu)$, ($\mu = \Omega, 0$), $k=0, \dots, 19$.

Using the functions $f_\mu(x)$, ($\mu = \Omega, 0$) and the field H_i , defined in the body text, the coefficients $A_k(\mu)$, ($\mu = \Omega, 0$), $k=0, \dots, 19$ for a layer i , are as follows :

$$A_0(\mu) = (1/2)^6 (f_\mu(6J+H_i) + 6f_\mu(4J+H_i) + 15f_\mu(2J+H_i) + 20f_\mu(H_i) + 15f_\mu(-2J+H_i) + 6f_\mu(-4J+H_i) + f_\mu(-6J+H_i))$$

$$A_1(\mu) = 4(1/2)^6 (f_\mu(6J+H_i) + 4f_\mu(4J+H_i) + 5f_\mu(2J+H_i) - 5f_\mu(-2J+H_i) - 4f_\mu(-4J+H_i) - f_\mu(-6J+H_i))$$

$$A_2(\mu) = 6(1/2)^6 (f_\mu(6J+H_i) + 2f_\mu(4J+H_i) - 2f_\mu(2J+H_i) - 4f_\mu(H_i) - f_\mu(-2J+H_i) + 2f_\mu(-4J+H_i) + f_\mu(-6J+H_i))$$

$$A_3(\mu) = 4(1/2)^6 (f_\mu(6J+H_i) - 3f_\mu(2J+H_i) + 3f_\mu(-2J+H_i) - f_\mu(-6J+H_i))$$

$$A_4(\mu) = (1/2)^6 (f_\mu(6J+H_i) - 2f_\mu(4J+H_i) - f_\mu(2J+H_i) + 4f_\mu(H_i) - f_\mu(-2J+H_i) - 2f_\mu(-4J+H_i) + f_\mu(-6J+H_i))$$

$$A_5(\mu) = (1/2)^6 (f_\mu(6J+H_i) + 4f_\mu(4J+H_i) + 5f_\mu(2J+H_i) - 5f_\mu(-2J+H_i) - 4f_\mu(-4J+H_i) - f_\mu(-6J+H_i))$$

$$A_6(\mu) = 4(1/2)^6 (f_\mu(6J+H_i) + 2f_\mu(4J+H_i) - f_\mu(2J+H_i) - 4f_\mu(H_i) - 5f_\mu(-2J+H_i) + 2f_\mu(-4J+H_i) + f_\mu(-6J+H_i))$$

$$A_7(\mu) = 6(1/2)^6 (f_\mu(6J+H_i) - 3f_\mu(2J+H_i) + 3f_\mu(-2J+H_i) - f_\mu(-6J+H_i))$$

$$A_8(\mu) = 4(1/2)^6 (f_\mu(6J+H_i) - 2f_\mu(4J+H_i) - f_\mu(2J+H_i) - 4f_\mu(H_i) - f_\mu(-2J+H_i) - 2f_\mu(-4J+H_i) + f_\mu(-6J+H_i))$$

$$A_9(\mu) = (1/2)^6 (f_\mu(6J+H_i) - 4f_\mu(4J+H_i) + 5f_\mu(2J+H_i) - 5f_\mu(-2J+H_i) + 4f_\mu(-4J+H_i) - f_\mu(-6J+H_i))$$

$$A_{10}(\mu) = (1/2)^6 (f_\mu(6J+H_i) + 4f_\mu(4J+H_i) + 5f_\mu(2J+H_i) - 5f_\mu(-2J+H_i) - 4f_\mu(-4J+H_i) - f_\mu(-6J+H_i))$$

$$A_{11}(\mu) = 4(1/2)^6 (f_\mu(6J+H_i) + 2f_\mu(4J+H_i) - f_\mu(2J+H_i) - 4f_\mu(H_i) - f_\mu(-2J+H_i) + 2f_\mu(-4J+H_i) + f_\mu(-6J+H_i))$$

$$A_{12}(\mu) = 6(1/2)^6 (f_\mu(6J+H_i) - 3f_\mu(2J+H_i) + 3f_\mu(-2J+H_i) - f_\mu(-6J+H_i))$$

$$A_{13}(\mu) = 4(1/2)^6 (f_\mu(6J+H_i) - 2f_\mu(4J+H_i)f_\mu(2J+H_i) + 4f_\mu(H_i) - f_\mu(-2J+H_i) - 2f_\mu(-4J+H_i) + f_\mu(-6J+H_i))$$

$$A_{14}(\mu) = (1/2)^6 (f_\mu(6J+H_i) - 4f_\mu(4J+H_i) + 5f_\mu(2J+H_i) - 5f_\mu(-2J+H_i) + 4f_\mu(-4J+H_i) - f_\mu(-6J+H_i))$$

$$A_{15}(\mu) = (1/2)^6 (f_\mu(6J+H_i) + 2f_\mu(4J+H_i) - f_\mu(2J+H_i) - 4f_\mu(H_i) - f_\mu(-2J+H_i) + 2f_\mu(-4J+H_i) + f_\mu(-6J+H_i))$$

$$A_{16}(\mu) = 4(1/2)^6 (f_\mu(6J+H_i) - 3f_\mu(2J+H_i) + 3f_\mu(-2J+H_i) - f_\mu(-6J+H_i))$$

$$A_{17}(\mu) = 6(1/2)^6 (f_\mu(6J+H_i) - 2f_\mu(4J+H_i) - f_\mu(2J+H_i) + 4f_\mu(H_i) - f_\mu(-2J+H_i) - 2f_\mu(-4J+H_i) + f_\mu(-6J+H_i))$$

$$A_{18}(\mu) = 4(1/2)^6 (f_\mu(6J+H_i) - 4f_\mu(4J+H_i) + 5f_\mu(2J+H_i) - 5f_\mu(-2J+H_i) + 4f_\mu(-4J+H_i) - f_\mu(-6J+H_i))$$

$$A_{19}(\mu) = (1/2)^6 (f_\mu(6J+H_i) - 6f_\mu(4J+H_i) + 15f_\mu(2J+H_i) - 20f_\mu(H_i) + 15f_\mu(-2J+H_i) - 6f_\mu(-4J+H_i) + f_\mu(-6J+H_i))$$