

Magnetic properties of mixed spin (1/2,1) Ising nanoparticles

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Abstract. Mixed spin 2D-nanoparticles (circle and square) with core – shell structure consisting of spin 1/2 and spin 1 distributed in concentric and two alternate rings are investigated by the use of the finite cluster approximation (FCA). In this approach, the state equations are derived. The effects of the exchange interactions on the phase diagrams are systematically discussed. A number of interesting phenomena have been found, in particular, the transition temperature is not too sensitive of shell exchange interaction where the spins S are strongly correlated.

1. Introduction

During the last few years, the research on magnetic nanomaterials such as nanoparticles, nanorods, nanobelts, nanowires and nanotubes, have been attracting considerable attention, and considered the most actively studied topics in statistical mechanics and condensed matter physics. The reason is due to their promising applications in nanotechnology [1,2] such as permanent magnets [3], information storage devices [4,5], biosensors [6] and some medical applications [7]. At present, the scientist can produce such kinds of fine nanoscaled materials [8,9], and the magnetization of certain nanomaterials such as γ -Fe₂O₃ nanoparticles has been experimentally measured [10]. In particular, magnetic nanowires and nanotubes such as ZnO [11], FePt, and Fe₃O₄ [12] can be synthesized by various experimental techniques and they have many applications in nanotechnology [13,14]. They are also utilized as raw materials in fabrication of ultra-high density magnetic recording media [15-17]. On the other hand, the magnetic properties of a nanometric scale material depend highly on the size and dimensionality of the nanomaterial.

From the theoretical point of view, Ising nanomagnetic systems have been studied by a variety of techniques, including mean field theory [18-20], effective field theory with correlations [21-24], Monte Carlo simulation [25-28], variational cumulant expansion method [29,30], and Green's function techniques [31].

Recently, the study of two sublattice mixed spin systems have become one of the actively studied subject in the statistical physics. They are of interest for the following main reasons. The first one is that they have less symmetry than their single-spin counterparts. The second one is that they are well adapted to study a certain type of ferrimagnetism [32], and finally many new phenomena are observed in these systems, which cannot be seen in the single-spin Ising model [33].

The aim of this paper is to investigate the mixed spin Ising nanoparticles. These latters, consisting of spin 1/2 and spin 1, have two different shapes (circle and square). In particular, we study the effect of the core and shell exchange interactions on the phase diagrams and the magnetizations. To this end,



we use the finite cluster approximation (FCA) [34,35] within the framework of a single-site cluster theory.

The outline of this work is as follows: in section 2, we present the model and the theoretical framework. The state equations are derived. The main results and discussion are arranged in section 3. Finally, the last section is devoted to a brief conclusion.

2. Theoretical framework

We consider two kinds of 2D-nanoparticles (circle and square), as depicted in figure 1. They are consisted of the surface shell and the core. The surface shell surrounds the core. Each site is occupied by an Ising spin where the σ and S spins are distributed in concentric and alternate rings.

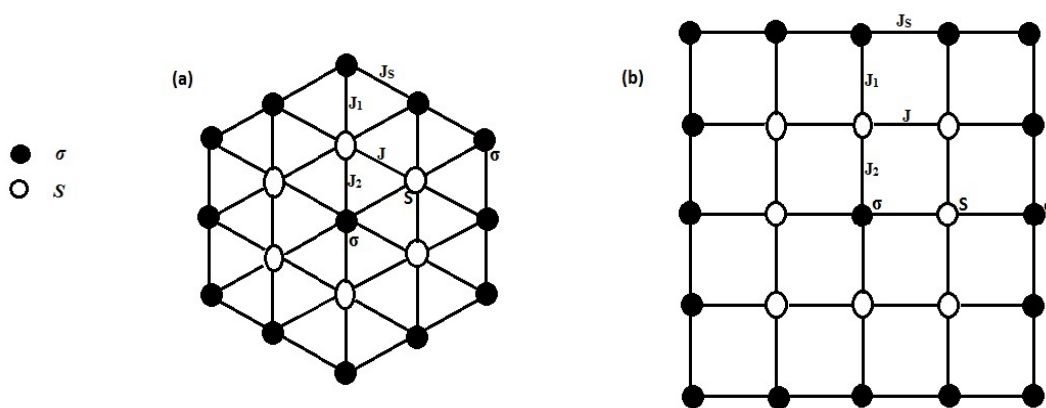


Figure 1. Schematic representations of two 2D-nanoparticles. They represent the circle nanoparticle (a) and the square nanoparticle (b). Atoms are denoted by σ_i (spin 1/2) and S_j (spin 1).

The Hamiltonian of the system is given by

$$H = -J_s \cdot \sum_{\langle i,j \rangle} \sigma_i \sigma_j - J \cdot \sum_{\langle m,n \rangle} S_m S_n - J_1 \cdot \sum_{\langle i,m \rangle} \sigma_i S_m - J_2 \cdot \sum_{\langle k,m \rangle} \sigma_k S_m \quad (1)$$

S_i and σ_j are the Pauli spin operators with $S=\pm 1, 0$ and $\sigma=\pm 1/2$. J_s is the exchange interaction between two nearest neighbor magnetic atoms at the surface shell. This latter is coupled to the next shell in the core with the exchange interaction J_1 . J is the exchange interaction between spins S_i in the core. J_2 is the exchange interaction between the central site σ_i and the sites S_i belonging to the first ring.

The method that we adopt in the study of the mixed spin Ising of nanoparticles (circle and square) consisting of spin 1/2 and spin 1 described by the Hamiltonian (1) is the finite cluster approximation (FCA) [34,35] based on a single-site cluster theory. We have to mention that this method has been successfully applied to a number of interesting pure and disordered spin Ising systems [36,39]. It has also been used for transverse Ising models [40-43] and semi-infinite Ising systems [44-48].

Within the core-shell concept, for the nanoparticle with a circle shape depicted in figure 1 (a), we have to determine the magnetizations at each site in the core and at the surface shell. Indeed, we denote by $\mu_3 = \langle \sigma_3 \rangle$, $m = \langle S \rangle$ the magnetizations per site in the core corresponding to the central site σ and the site belonging to the ring consisting by spin S , respectively. At the surface shell of the system,

we have to define two magnetizations $\mu_1 = \langle \sigma_1 \rangle$ and $\mu_2 = \langle \sigma_2 \rangle$ which correspond to the coordination numbers $z=3$ and $z=4$, respectively.

We split the total Hamiltonian (1) into two parts, $H = H_0 + H'$ where H_0 includes all parts of H associated with the lattice site 0. In the present system, H_0 takes the form

$$H_{0\sigma_1} = -[J_S \cdot (\sigma_{2,1} + \sigma_{2,2}) + J \cdot S_1] \cdot \sigma_{1,0} \quad (2)$$

$$H_{0\sigma_2} = -[J_S \cdot (\sigma_{1,1} + \sigma_{1,2}) + J_1 \cdot (S_1 + S_2)] \cdot \sigma_{2,0} \quad (3)$$

$$H_{0\sigma_3} = -[J_2 \cdot \sum_{i=1}^6 S_i] \cdot \sigma_{3,0} \quad (4)$$

$$H_{0S} = -[J \cdot (S_1 + S_2) + J_1 \cdot (\sigma_{1,1} + \sigma_{2,1} + \sigma_{2,2}) + J_2 \cdot \sigma_3] \cdot S_0 \quad (5)$$

Whether the lattice site 0 belongs to σ or S -sublattice, respectively.

Using the framework of the FCA, we evaluate $\langle \sigma_{1,0} \rangle_c$, $\langle \sigma_{2,0} \rangle_c$, $\langle \sigma_{3,0} \rangle_c$ and $\langle (S_0)^n \rangle_c$ ($n=1, 2$) the mean values of $\sigma_{1,0}$, $\sigma_{2,0}$, $\sigma_{3,0}$, $(S_0)^n$ for a given configuration c of all other spins (i.e when all other spins σ_i and S_j are kept fixed).

$\langle \sigma_{1,0} \rangle_c$, $\langle \sigma_{2,0} \rangle_c$, $\langle \sigma_{3,0} \rangle_c$ and $\langle (S_0)^n \rangle_c$ are given by

$$\langle \sigma_{1,0} \rangle_c = \frac{\text{Tr}_{\sigma_{1,0}}(\sigma_{1,0} \cdot \exp(-\beta \cdot H_{0\sigma_1}))}{\text{Tr}_{\sigma_{1,0}}(\exp(-\beta \cdot H_{0\sigma_1}))} \quad (6)$$

$$\langle \sigma_{2,0} \rangle_c = \frac{\text{Tr}_{\sigma_{2,0}}(\sigma_{2,0} \cdot \exp(-\beta \cdot H_{0\sigma_2}))}{\text{Tr}_{\sigma_{2,0}}(\exp(-\beta \cdot H_{0\sigma_2}))} \quad (7)$$

$$\langle \sigma_{3,0} \rangle_c = \frac{\text{Tr}_{\sigma_{3,0}}(\sigma_{3,0} \cdot \exp(-\beta \cdot H_{0\sigma_3}))}{\text{Tr}_{\sigma_{3,0}}(\exp(-\beta \cdot H_{0\sigma_3}))} \quad (8)$$

$$\langle S_0^n \rangle_c = \frac{\text{Tr}_{S_0}(S_0^n \cdot \exp(-\beta \cdot H_{0S}))}{\text{Tr}_{S_0}(\exp(-\beta \cdot H_{0S}))} \quad (9)$$

Here, Tr_{σ_0} (Tr_{S_0} or) means the trace performed over σ_0 (or S_0). As usual $\beta=1/T$, where T is the absolute temperature. $n=1,2$ correspond to the magnetization and the quadrupolar moment respectively. Therefore, the magnetizations at the shell and in the core are then given by

$$\mu_1 = \langle \langle \sigma_{1,0} \rangle_c \rangle = \left\langle \frac{\text{Tr}_{\sigma_{1,0}}(\sigma_{1,0} \cdot \exp(-\beta \cdot H_{0\sigma_1}))}{\text{Tr}_{\sigma_{1,0}}(\exp(-\beta \cdot H_{0\sigma_1}))} \right\rangle \quad (10)$$

$$\mu_2 = \langle \langle \sigma_{2,0} \rangle_c \rangle = \left\langle \frac{\text{Tr}_{\sigma_{2,0}}(\sigma_{2,0} \cdot \exp(-\beta \cdot H_{0\sigma_2}))}{\text{Tr}_{\sigma_{2,0}}(\exp(-\beta \cdot H_{0\sigma_2}))} \right\rangle \quad (11)$$

$$\mu_3 = \langle \langle \sigma_{3,0} \rangle_c \rangle = \left\langle \frac{\text{Tr}_{\sigma_{3,0}}(\sigma_{3,0} \cdot \exp(-\beta \cdot H_{0\sigma_3}))}{\text{Tr}_{\sigma_{3,0}}(\exp(-\beta \cdot H_{0\sigma_3}))} \right\rangle \quad (12)$$

$$m = \langle \langle S_0 \rangle_c \rangle = \left\langle \frac{\text{Tr}_{S_0}(S_0 \cdot \exp(-\beta \cdot H_{0S}))}{\text{Tr}_{S_0}(\exp(-\beta \cdot H_{0S}))} \right\rangle \quad (13)$$

$$q = \langle \langle S_0^2 \rangle_c \rangle = \left\langle \frac{\text{Tr}_{S_0}(S_0^2 \cdot \exp(-\beta \cdot H_{0S}))}{\text{Tr}_{S_0}(\exp(-\beta \cdot H_{0S}))} \right\rangle \quad (14)$$

where $\langle \dots \rangle$ denotes the average over all spin configurations. q is the quadrupolar moment. Performing the inner traces in (10)-(14) over the states of the selected σ_0 spin (S_0), we obtain the following exact relations

$$\mu_1 = \left\langle \frac{1}{2} \tanh \left[\frac{K}{2} \{ \alpha_2 \cdot (\sigma_{2,1} + \sigma_{2,2}) + \alpha_1 \cdot S_1 \} \right] \right\rangle \quad (15)$$

$$\mu_2 = \left\langle \frac{1}{2} \tanh \left[\frac{K}{2} \{ \alpha_2 \cdot (\sigma_{1,1} + \sigma_{1,2}) + \alpha_1 \cdot (S_1 + S_2) \} \right] \right\rangle \quad (16)$$

$$\mu_3 = \left\langle \frac{1}{2} \tanh \left[\frac{K}{2} \{ S_1 + S_2 + S_3 + S_4 + S_5 + S_6 \} \right] \right\rangle \quad (17)$$

$$m = \left\langle \frac{2 \sinh [K \{ \alpha_1 \cdot (\sigma_1 + \sigma_{2,1} + \sigma_{2,2}) + \sigma_3 + \alpha_3 \cdot (S_1 + S_2) \}]}{1 + 2 \cosh [K \{ \alpha_1 \cdot (\sigma_1 + \sigma_{2,1} + \sigma_{2,2}) + \sigma_3 + \alpha_3 \cdot (S_1 + S_2) \}]} \right\rangle \quad (18)$$

$$q = \left\langle \frac{2 \cosh [K \{ \alpha_1 \cdot (\sigma_1 + \sigma_{2,1} + \sigma_{2,2}) + \sigma_3 + \alpha_3 \cdot (S_1 + S_2) \}]}{1 + 2 \cosh [K \{ \alpha_1 \cdot (\sigma_1 + \sigma_{2,1} + \sigma_{2,2}) + \sigma_3 + \alpha_3 \cdot (S_1 + S_2) \}]} \right\rangle \quad (19)$$

where $K = \beta J_2$, $\alpha_1 = J_1/J_2$, $\alpha_2 = J_s/J_2$ and $\alpha_3 = J/J_2$.

Now, we have to average the right-hand sides of Eqs. (15)-(19) over all spin configurations, within the FCA framework. This latter has been designed to treat all spin self-correlations exactly while still neglecting correlations between different spins. We can easily observe that any functions such as $f(\sigma, S)$ and $g(S)$ of σ and S can be written as the linear superposition

$$f(\sigma, S) = f_1 + f_2 \cdot \sigma + f_3 \cdot S + f_4 \cdot S^2 + f_5 \cdot \sigma \cdot S + f_6 \cdot \sigma \cdot S^2 \quad (20)$$

$$g(S) = g_1 + g_2 \cdot S + g_3 \cdot S^2 \quad (21)$$

with appropriate coefficients $f_i (i=1, \dots, 6)$ and $g_j (j=1, 2, 3)$. Applying this to all spins σ_i and S_j in expressions between brackets in Eqs. (15)-(19), we obtain

$$\langle \sigma_{1,0} \rangle_c = \sum_{p=0}^2 \sum_{n=0}^1 \sum_{\ell=0}^{1-n} \sum_{i=1}^2 A_i^{p,n,\ell} [\sigma_i S_m S_m^2] \quad (22)$$

$$\langle \sigma_{2,0} \rangle_c = \sum_{p=0}^2 \sum_{n=0}^2 \sum_{\ell=0}^{2-n} \sum_{i=1}^2 \sum_{j=1}^2 \sum_{\substack{k=1 \\ (k \neq j)}}^2 B_{i,j,k}^{p,n,\ell} [\sigma_i S_j S_k^2] \quad (23)$$

$$\langle \sigma_{3,0} \rangle_c = \sum_{n=0}^6 \sum_{\ell=0}^{6-n} \sum_{i=1}^6 \sum_{\substack{j=1 \\ j \neq i}}^6 C_{i,j}^{n,\ell} [S_i S_j^2] \quad (24)$$

$$\langle S_0 \rangle_c = \sum_{p=0}^4 \sum_{n=0}^2 \sum_{\ell=0}^{2-n} \sum_{i=1}^4 \sum_{j=1}^2 \sum_{\substack{k=1 \\ k \neq j}}^2 D_{i,j,k}^{p,n,\ell} [\sigma_i S_j S_k^2] \quad (25)$$

$$\langle S_0^2 \rangle_c = \sum_{p=0}^4 \sum_{n=0}^2 \sum_{\ell=0}^{2-n} \sum_{i=1}^4 \sum_{j=1}^2 \sum_{\substack{k=1 \\ k \neq j}}^2 E_{i,j,k}^{p,n,\ell} [\sigma_i S_j S_k^2] \quad (26)$$

where $[\sigma_i S_j (S_k)^2]$ denotes the term containing p different factors of σ_i , n different factors of S_j , and ℓ different factors of $(S_k)^2$ with $(k \neq j)$. $[S_j (S_k)^2]$ denotes the term containing n different factors of S_j , and ℓ different factors of $(S_k)^2$. These factors are selected from sets $\{\sigma_1, \sigma_2, S_m\}$, $\{\sigma_1, \sigma_2, S_1, S_2\}$, $\{S_1, S_2, S_3, S_4, S_5, S_6\}$ and $\{\sigma_1, \sigma_2, \sigma_3, \sigma_4, S_1, S_2\}$ for $\langle \sigma_{1,0} \rangle_c$, $\langle \sigma_{2,0} \rangle_c$, $\langle \sigma_{3,0} \rangle_c$ and $\langle (S_0)^n \rangle_c$, respectively.

For example:

- $p=1, n=0, \ell=1$: $A_i^{p,n,\ell} \sigma_i S_m S_m^2 = A_1^{1,0,1} \sigma_1 S_m^2$
- $p=2, n=1, \ell=1$: $B_{i,j,k}^{p,n,\ell} \sigma_i S_j S_k^2 = B_{(1,2),1,2}^{2,1,1} \sigma_1 \sigma_2 S_1 S_2^2$
- $n=3, \ell=1$: $C_{i,j}^{n,\ell} S_i S_j^2 = C_{(1,2,3),5}^{3,1} S_1 S_2 S_3 S_5^2$

The magnetizations at the shell and in the core are given by Eqs. (15)-(19) using the expansions (22)-(26). They constitute a set of exact relations according to which we can study the nanoparticle with a circle shape. However, in order to carry out the thermal average over all spin configurations, we have to deal with multispin correlations appearing via the right-hand side of Eqs. (22)-(26). The problem becomes mathematically intractable if we try to treat them exactly in the spirit of the FCA. In this paper, we use the simplest approximation in which we treat all spin self-correlations exactly while still neglecting correlations between quantities pertaining to different sites. This leads to the following coupled equations

$$\mu_1 = \mu_2 \cdot (2A_1 + 2A_3 \cdot q) + m \cdot A_2 + \mu_2^2 \cdot m \cdot A_4 \quad (27)$$

$$\mu_2 = \mu_1 \cdot (2B_1 + 4B_3 \cdot q + 2B_7 \cdot q^2) + m \cdot (2B_2 + 2B_6 \cdot q) + m \cdot \mu_1^2 \cdot (2B_4 + 2B_8 \cdot q) + 2 \cdot B_5 \cdot m^2 \cdot \mu_1 \quad (28)$$

$$\mu_3 = m \cdot (6C_1 + 30C_2 \cdot q + 60C_3 \cdot q^2 + 60C_4 \cdot q^3 + 30C_5 \cdot q^4 + 6C_6 \cdot q^5) + m^3 \cdot (20C_7 + 60C_8 \cdot q + 60C_9 \cdot q^2 + 20C_{10} \cdot q^3) + m^5 \cdot (6C_{11} + 6C_{12} \cdot q) \quad (29)$$

$$\begin{aligned} m = & \mu_1 \cdot (D_1 + 2D_{10} \cdot q + D_{21} \cdot q^2) + \mu_2 \cdot (2D_1 + 4D_{10} \cdot q + 2D_{21} \cdot q^2) + \mu_3 \cdot (D_2 + 2D_{11} \cdot q + \\ & D_{22} \cdot q^2) + m \cdot (2D_3 + 2D_4 \cdot q) + \mu_1 \cdot \mu_2^2 \cdot (D_5 + 2D_{12} \cdot q + D_{24} \cdot q^2) + \mu_3 \cdot \mu_2^2 \cdot (D_6 + 2D_{13} \cdot q + \\ & D_{23} \cdot q^2) + m \cdot \mu_2^2 \cdot (2D_7 + 2D_{18} \cdot q) + \mu_1 \cdot m^2 \cdot (D_{14}) + \mu_2 \cdot m^2 \cdot (2D_{14}) + \mu_3 \cdot m^2 \cdot (D_{15}) + \\ & \mu_1 \cdot \mu_2 \cdot \mu_3 \cdot (2D_6 + 4D_{13} \cdot q + 2D_{23} \cdot q^2) + m \cdot \mu_1 \cdot \mu_2 \cdot (4D_7 + 4D_{18} \cdot q) + m \cdot \mu_1 \cdot \mu_3 \cdot (2D_8 + 2D_{19} \cdot q) + \\ & m \cdot \mu_2 \cdot \mu_3 \cdot (4D_8 + 4D_{19} \cdot q) + m \cdot \mu_1 \cdot \mu_3 \cdot \mu_2^2 \cdot (2D_9 + 2D_{20} \cdot q) + \mu_1 \cdot m^2 \cdot \mu_2^2 \cdot (D_{16}) + \mu_3 \cdot m^2 \cdot \mu_2^2 \cdot (D_{17}) + \\ & \mu_1 \cdot \mu_2 \cdot \mu_3 \cdot m^2 \cdot (2D_{17}) \end{aligned} \quad (30)$$

$$\begin{aligned} q = & (E_1 + 2E_5 \cdot q + E_7 \cdot q^2) + \mu_2^2 \cdot (E_2 + 2E_{12} \cdot q + E_{22} \cdot q^2) + \mu_1 \cdot \mu_2 \cdot (2E_2 + 4E_{12} \cdot q + 2E_{22} \cdot q^2) + \\ & \mu_1 \cdot \mu_3 \cdot (E_3 + 2E_{13} \cdot q + E_{23} \cdot q^2) + \mu_2 \cdot \mu_3 \cdot (2E_3 + 4E_{13} \cdot q + 2E_{23} \cdot q^2) + m^2 \cdot (E_6) + m \cdot \mu_1 \cdot (2E_8 + \\ & 2E_{18} \cdot q) + m \cdot \mu_2 \cdot (4E_8 + 4E_{18} \cdot q) + m \cdot \mu_3 \cdot (2E_9 + 2E_{19} \cdot q) + \mu_1 \cdot \mu_3 \cdot \mu_2^2 \cdot (E_4 + 2E_{14} \cdot q + E_{24} \cdot q^2) + \\ & \mu_1 \cdot \mu_2 \cdot \mu_3 \cdot m \cdot (4E_{10} + 4E_{21} \cdot q) + m \cdot \mu_1 \cdot \mu_2^2 \cdot (2E_{11} + 2E_{20} \cdot q) + m \cdot \mu_3 \cdot \mu_2^2 \cdot (2E_{10} + 2E_{21} \cdot q) + \\ & \mu_1 \cdot \mu_2 \cdot m^2 \cdot (2E_{16}) + \mu_1 \cdot \mu_3 \cdot m^2 \cdot (E_{17}) + \mu_2 \cdot \mu_3 \cdot m^2 \cdot (2E_{17}) + m^2 \cdot \mu_2^2 \cdot (E_{16}) + m^2 \cdot \mu_2^2 \cdot \mu_1 \cdot \mu_3 \cdot (E_{15}) \end{aligned} \quad (31)$$

The non-zero coefficients quoted in Eqs. (27)-(31), are listed in the appendix.

If we substitute μ_i ($i=1,2,3$) and q into (30) with their expressions taken from (27), (28), (29) and (31), we obtain an equation for m of the form

$$m = a \cdot m + b \cdot m^3 + \dots \quad (32)$$

The second-order transition is determined by the condition $a=1$. For this reason, we neglect higher-order terms in the magnetizations in (27)-(31). Therefore, the transition temperature is analytically determined by the equation

$$1 = 2D_3 + 2D_4 \cdot q_0 + (D_1 + 2D_{10} \cdot q_0 + D_{21} \cdot q_0^2) \cdot (A + 2B) + C \cdot (D_2 + 2D_{11} \cdot q_0 + D_{22} \cdot q_0^2) \quad (33)$$

where q_0 is the solution of

$$q_0 = E_1 + 2E_5 \cdot q_0 + E_7 \cdot q_0^2 \quad (34)$$

Eq. (33) means that the right-hand-side corresponds to the coefficient a in Eq. (32).

The magnetization m in the vicinity of the second-order transition is given by

$$m^2 = \frac{1-a}{b} \quad (35)$$

The right-hand side of (35) must be positive. If this is not the case, the transition is of the first-order and the point at which $a=1$ and $b=0$ characterizes the tricritical point.

To obtain the expression for b , one has to solve Eqs (27)-(31) for small μ_1 , μ_2 , μ_3 and m . The solution is of the form

$$q = q_0 + q_1 \cdot \mu_2^2 + q_2 \cdot m^2 + q_3 \cdot \mu_1 \cdot m + q_4 \cdot \mu_2 \cdot m + q_5 \cdot \mu_3 \cdot m + q_6 \cdot \mu_1 \cdot \mu_2 + q_7 \cdot \mu_1 \cdot \mu_3 + q_8 \cdot \mu_2 \cdot \mu_3 \quad (36)$$

After some algebraic manipulations, Eqs (27), (28), (29) and (36) can be written in the following forms

$$\mu_1 = A \cdot m + D \cdot m^3 + \dots \quad (37)$$

$$\mu_2 = B \cdot m + E \cdot m^3 + \dots \quad (38)$$

$$\mu_3 = C \cdot m + F \cdot m^3 + \dots \quad (39)$$

$$q = q_0 + q_9 \cdot m^2 \quad (40)$$

By substituting μ_1 , μ_2 , μ_3 and q in Eq.(30), with their expressions taken from (37)-(40), we obtain the equation (32), where b is given by

$$b = D_1 \cdot (2E + D) + D_2 \cdot F + 2D_4 \cdot q_9 + D_5 \cdot A \cdot B^2 + D_6 \cdot (C \cdot B^2 + 2A \cdot B \cdot C) + D_7 \cdot (4A \cdot B + 2B^2) + D_8 \cdot (4B \cdot C + 2A \cdot C) + D_{10} \cdot (4q_0 \cdot E + 4q_9 \cdot B + 2q_0 \cdot D + 2q_9 \cdot A) + 2D_{11} \cdot (q_0 \cdot F + q_9 \cdot C) + 2D_{12} \cdot q_0 \cdot A \cdot B^2 + D_{13} \cdot (4q_0 \cdot A \cdot B \cdot C + 2q_0 \cdot B^2 \cdot C) + D_{14} \cdot (2B + A) + D_{15} \cdot C + D_{18} \cdot (2q_0 \cdot B^2 + 4q_0 \cdot A \cdot B) + D_{19} \cdot (4q_0 \cdot B \cdot C + 2q_0 \cdot A \cdot C) + D_{21} \cdot (2q_0 \cdot q_9 \cdot A + q_0^2 \cdot D + 2q_0^2 \cdot E + 4q_0 \cdot q_9 \cdot B) + D_{22} \cdot (q_0^2 \cdot F + 2q_0 \cdot q_9 \cdot C) + D_{23} \cdot (q_0^2 \cdot B^2 \cdot C + 2q_0^2 \cdot A \cdot B \cdot C) + D_{24} \cdot q_0^2 \cdot A \cdot B^2 \quad (41)$$

For the nanoparticle with a square shape depicted in figure 1(b), we define three magnetizations μ_1 , μ_2 , μ_3 at the surface shell, three magnetizations (m_1 and m_2 at the second shell and μ_4 at the center) in the core, and two quadrupolar moments q_1 and q_2 . Using FCA, we determine all these quantities from coupled equations, similar to those (Eqs. (27)-(31)) written for the circle nanoparticle. They will not be presented here.

3. Results and discussion

Let us introduce the magnetizations m_{sh} and m_C at the shell and in the core as well as the total magnetization per site m_T . Their expressions are given by

$$m_{sh} = \frac{\mu_1 + \mu_2}{2}, \quad m_C = \frac{\mu_3 + 6m}{7}, \quad m_T = \frac{6\mu_1 + 6\mu_2 + \mu_3 + 6m}{19} \quad (42)$$

for circle nanoparticle

$$m_{sh} = \frac{\mu_1 + 2\mu_2 + \mu_3}{4}, \quad m_C = \frac{\mu_4 + 4m_1 + 4m_2}{9}, \quad m_T = \frac{4\mu_1 + 8\mu_2 + 4\mu_3 + \mu_4 + 4m_1 + 4m_2}{25} \quad (43)$$

for square nanoparticle

In this section, we study the effects of core and shell couplings on the phase diagrams of the circle and square 2D-nanoparticles. In the following discussions, all interactions as well as the temperature are normalized with exchange interaction J_2 between the central site and the sites belonging to the outer boundary of the core. In the present work, we consider that the shells at the surface and in the core interact with each other via the same coupling ($J_1=J_2$).

In order to examine the transition temperature of the shell and the core, we investigate the thermal dependence of the magnetizations. Firstly, we can see from figure 2 and figure 3 that all magnetizations (μ_1 , μ_2 , μ_3 and m) decrease to zero continuously as the temperature increases; therefore, a second-order phase transition occurs. On the other hand, by analyzing the coupled equations (27)-(31), we find that all magnetizations vanish at a unique transition temperature, which is solution of Eq. (33). This behavior is observed for any strength of the Hamiltonian parameters as is shown in figure 2 and figure 3. Therefore, the shell and the core undergo a transition at the same temperature. Further, we note from these figures that the core exchange interaction J has the effect of increasing the critical temperature. In other words, the long-range ferromagnetic order domain becomes more and more wider with increasing values of exchange interaction J . The same behaviors are also observed for the nanoparticle with square shape.

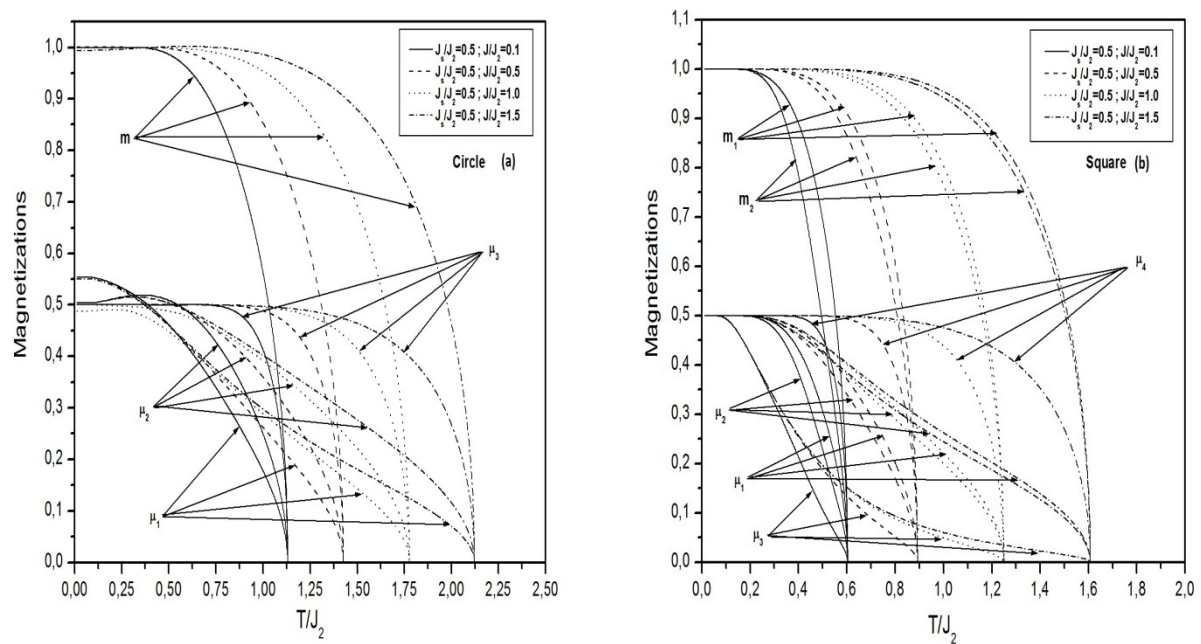


Figure 2. The thermal dependence of the magnetizations (μ and m) for selected values of J s and J . (a) circle nanoparticle and (b) square nanoparticle.

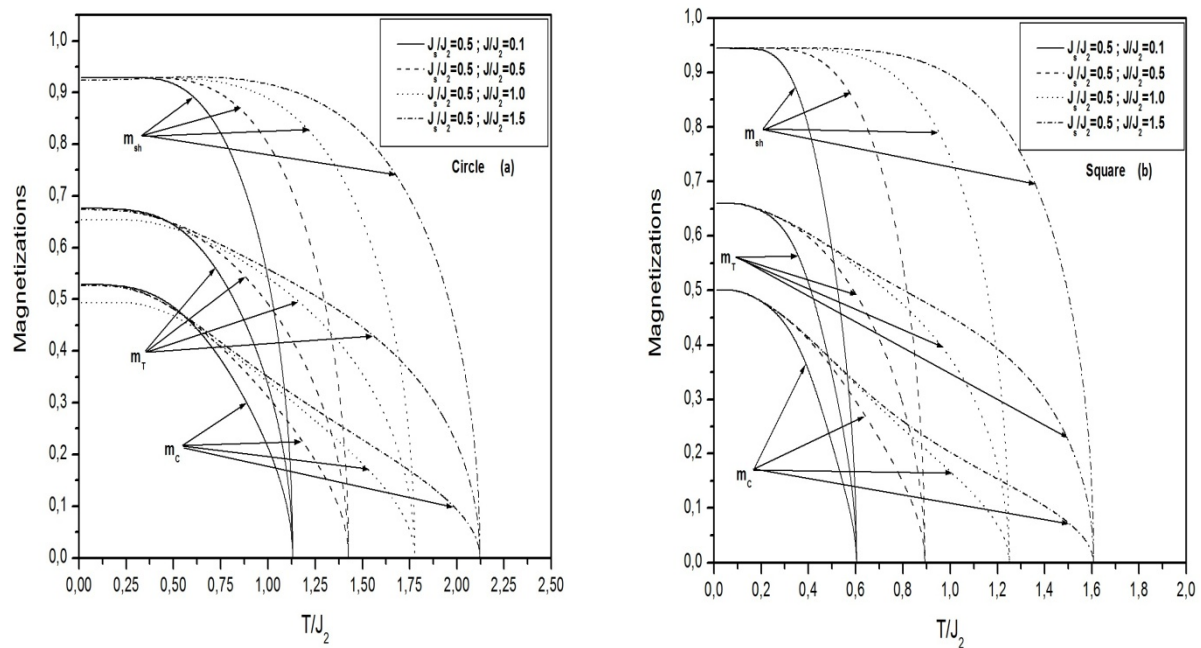


Figure 3. The thermal dependence of the magnetizations at the shell m_{sh} , in the core m_c and the total magnetization m_T , for selected values of J_s and J . (a) circle nanoparticle and (b) square nanoparticle.

In figure 4, we present in $(T_c/J_2, J/J_2)$ plane the phase diagrams for circle and square nanoparticles for selected values of the shell coupling J_s . As seen in this figure, for fixed value of the shell coupling J_s , the transition temperature increases gradually with the increase of J . For relatively low strength of this latter interaction, the transition temperature increases with J_s . This dependence becomes less and less sensitive for high values of the surface exchange interaction. In other word, for important values of J the ferromagnetic order of the core coupling are dominant against the shell coupling J_s , hence the transition temperature of the system becomes independent of shell coupling J_s . We note that this behavior is more pronounced for the nanoparticle with a square shape. Indeed, the positive value of the exchange interaction J rises the absolute value of lattice energy coming from the spin1-spin1 interaction, and then reinforce the longitudinal magnetization. Therefore it acts in favor of the order. Thus the domain of the order state becomes wider and the transition temperature increases with J . On the other hand, one should notice that the transition temperature of circle nanoparticle is greater than the one of square nanoparticle. This is because the difference of the atomic arrangement, namely the atomic arrangement in the circle is more closely packed than the one in the square. The similar phenomena have also been observed in the phase diagrams of a nanowire and a nanotube [22].

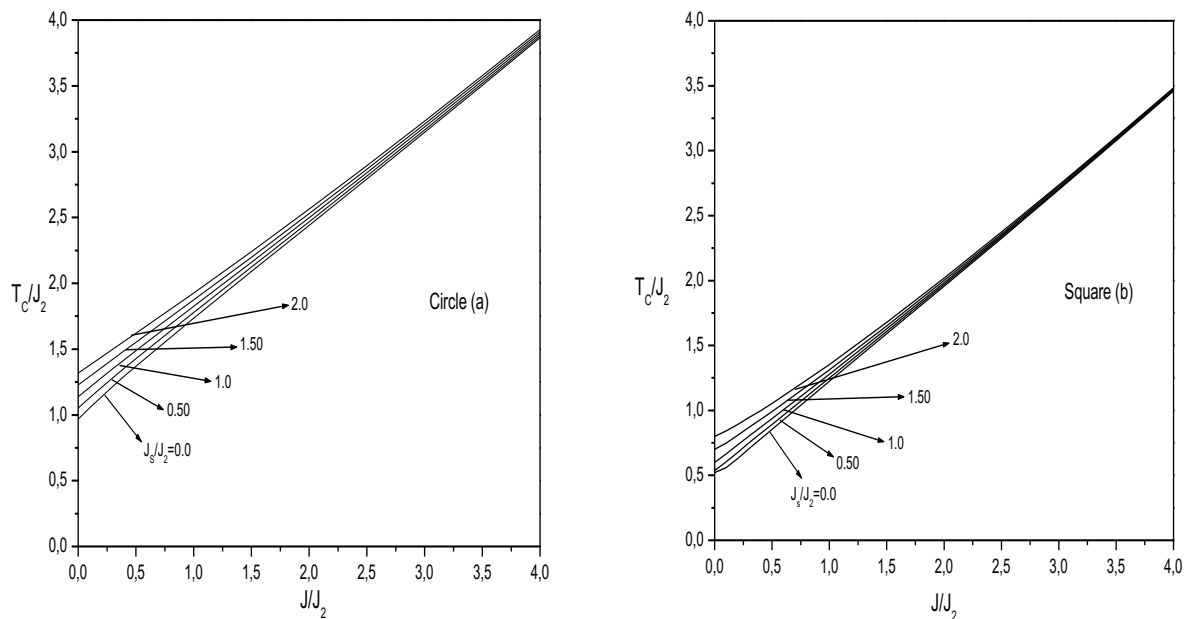


Figure 4. The phase diagrams in the $(T_c/J_2, J/J_2)$ plane of the two nanoparticles, (a) the circle nanoparticle and (b) the square nanoparticle. The number accompanying each curve denotes the value of J_s/J_2 .

4. Conclusion

In this work, we have studied the magnetic properties of the mixed spin Ising 2D-nanoparticles (circle and square) formed by alternate layers of σ and S spins using the finite cluster approximation (FCA) within the single-cluster theory. Let summarize by stating the main results of this investigation.

Firstly, we have reported the effects of the exchange interaction between spins S and the shell coupling on the phase diagrams, it has been shown that the increasing values of J_s and J interaction increase the transition temperature. This latter becomes not so sensitive of shell exchange interaction where the spins S are strongly correlated.

Secondly, the thermal behaviours of the longitudinal magnetizations have also been examined. It has been found that all sublattice magnetizations vanish at a unique transition temperature for any strength of the hamiltonian parameters Therefore the shell and the core undergo a transition at the same temperature.

References

- [1] Kim T Y, Yamazaki Y and Hirano T 2004 *Phys. Status Solidi B* **241** 1601
- [2] Kodama R H 1999 *J. Magn. Magn. Mater.* **200** 359
- [3] Zeng H, Li J, Liu J P, Wang Z L and Sun S 2002 *Nature* **420** 395
- [4] Hayashi T, Hirono S, Tomita M and Umemura S 1996 *Nature* **381** 772
- [5] Kodama R H, Berkowitz J A E, McNiff E J and Foner J S 1996 *Phys. Rev. Lett.* **774** 394
- [6] Kurlyandskaya G V, Sanchez M L, Hernando B, Prida V M, Gorria P and M. Tejedor 2003 *Appl. Phys. Lett.* **82** 3053
- [7] Alexiou C, Schmidt A, Klein R, Hullin P, Bergemann C and Arnold W 2002 *J. Magn. Magn. Mater.* **252** 363
- [8] Ruhrig M, Khamsehpour B, Kirk K J, Chapman J N, Aitchison P, McVitie S and Wilkinsons C D W 1996 *IEEE Trans. Magn.* **32** 4452
- [9] Scherfl T, Fidler J, Kirk K J and Chapman J N 1997 *J. Magn. Magn. Mater.* **175** 193
- [10] Martinez B, Obradors X, Balcells L, Rouanet A and Monty C 1998 *Phys. Rev. Lett.* **80** 181
- [11] Fan Z and LU J G 2006 *Int. J. High speed Electron. Systems* **16** 883
- [12] Su Y C, Skomski R, Sorge K D and Sellmyer D J 2004 *Appl. Phys. Lett.* **84** 1525
- [13] Skomski R 2003 *J. Phys. Condens. Matter* **15** R841.
- [14] Schlörb H, Haehnel V, Khatri M S, Srivastav A, Kumar A, Schultz L and Fähler S 2010 *Phys. Status solidi B* **247** 2364
- [15] Wegrove J E, Kelly D, Jaccard Y, Guittienne Ph and Ansermet J –Ph 1999 *Europhys. Lett.* **45** 626.
- [16] Fert A and Piraux L 1999 *J. Magn. Magn. Mater.* **200** 338.
- [17] Bader S D 2006 *Rev. Mod. Phys.* **78** 1
- [18] Leite V S and Figueiredo W 2005 *Physica A* **350** 379
- [19] Kaneyoshi T 2009 *Phys. Status Solidi B* **246** 2359
- [20] Michael F, Gonzalez C, Mujica V, Marquez M and Ratner A M 1996 *Phys. Rev. B* **76** 224409
- [21] Kaneyoshi T 2011 *J. Magn. Magn. Mater.* **323** 1145
- [22] Kaneyoshi T 2011 *Phys. Status Solidi B* **248** 250
- [23] Sarli N and Keskin M 2012 *Solid State Commun.* **152** 354
- [24] Canko O, Erdinç A, Taskin F and Yildirim A F 2012 *J. Magn. Magn. Mater.* **324** 508
- [25] Vasilakaki M and Trohidou K N 2009 *Phys. Rev. B* **79** 144402
- [26] Zaim A, Kerouad M and Y. El Amraoui Y 2009 *J. Magn. Magn. Mater.* **321** 1083
- [27] Eglesias O, Battle X and Labarta A 2007 *J. Phys. Condens. Matter* **19** 406232
- [28] Eglesias O, Battle X and Labarta A 2005 *Phys. Rev. B* **72** 212401
- [29] Wang H, Zhou Y, Lin D L and Wang C 2002 *Phys. Status Solidi B* **232** 254
- [30] Wang H, Zhou Y, Wang E and Lin D L 2001 *Chin. J. Phys.* **39** 85
- [31] Garanin D A and Kachkachi H 2003 *Phys. Rev. Lett.* **90** 65504
- [32] Néel L 1948 *Ann. Phys. (Paris)* **3** 137
- [33] Albayrak E and Keskin M 2003 *J. Magn. Magn. Mater.* **261** 196
- [34] Boccara N 1983 *Phys. Lett A* **94** 185
- [35] Benyoussef A and Boccara N 1983 *J. Phys.* **44** 1143.
- [36] Benayad N, Clümper A, Zittartz J and Benyoussef A 1989 *Z. Phys. B* **77** 339
- [37] Benayad N, Dakhama A, Clümper A and Zittartz J 1996 *Ann. Phys. Lpz.* **5** 387
- [38] Benayad N, Khaya L and Fathi A 2002 *J. Phys. Condens. Matter.* **14** 9667
- [39] Benayad N, Fathi A and Khaya L 2001 *Physica A* **300** 225
- [40] Benayad N, Zerhouni R and Clümper A 1998 *Eur. Phys. J. B* **5** 687
- [41] Benayad N, Fathi A and Khaya L 2004 *J. Magn. Magn. Mater.* **278** 407
- [42] Benayad N, Fathi A and Zerhouni R 2000 *J. Magn. Magn. Mater.* **222** 355
- [43] Benyoussef A and Ez-Zahraoui H 1994 *J. Phys. Condens. Matter.* **6** 3411
- [44] Lahcini T and Benayad N 2009 *Phase Transitions* **82** 197

- [45] Khaya L, Benayad N and Dakhama A 2004 *Phys Status Solidi B* **241** 1078
- [46] Benayad N and Dakhama A 1997 *Phys. Rev B* **55** 12276
- [47] Benayad N and Dakhama A 1997 *J. Magn. Magn. Mater.* **168** 105
- [48] Benyoussef A, Boccara N and Saber M 1985 *J. Phys C* **18** 4275

Appendix

The coefficients $A_i(i=1,\dots,4)$, $B_i(i=1,\dots,8)$, $C_i(i=1,\dots,12)$, $D_i(i=1,\dots,24)$ and $E_i(i=1,\dots,24)$ appearing respectively in eqs. (27), (28), (29), (30) and (31), also the coefficients A , B , C , D , E , F , q_1 , q_2 , q_3 , q_4 , q_5 , q_6 , q_7 , q_8 and q_9 are given by:

For abbreviation we consider new functions

$$f(x) = \frac{1}{2} \tanh\left(\frac{\beta}{2}x\right)$$

$$F_1(x) = \frac{2\sinh(\beta x)}{1+2\cosh(\beta x)}$$

$$F_2(x) = \frac{2\cosh(\beta x)}{1+2\cosh(\beta x)}$$

$$A_1 = f(J_s)$$

$$A_2 = \frac{1}{4}f(J_s + J_1) - \frac{1}{4}f(J_s - J_1) + \frac{1}{2}f(J_1)$$

$$A_3 = \frac{1}{2}f(J_s + J_1) + \frac{1}{2}f(J_s - J_1) - f(J_s)$$

$$A_4 = f(J_s + J_1, \Omega_s) - f(J_s - J_1) - 2f(J_1)$$

$$B_1 = f(J_s,)$$

$$B_2 = \frac{1}{4}f(J_s + J_1) - \frac{1}{4}f(J_s - J_1) + \frac{1}{2}f(J_1)$$

$$B_3 = \frac{1}{2}f(J_s + J_1) + \frac{1}{2}f(J_s - J_1) - f(J_s)$$

$$B_4 = f(J_s + J_1) - f(J_s - J_1) - 2.f(J_1)$$

$$B_5 = \frac{1}{4}f(J_s + 2J_1) + \frac{1}{4}f(J_s - 2J_1) - \frac{1}{2}f(J_s)$$

$$B_6 = \frac{1}{8}f(J_s + 2J_1, \Omega_s) - \frac{1}{8}f(J_s - 2J_1) - \frac{1}{4}f(J_s + J_1) + \frac{1}{4}f(J_s - J_1) + \frac{1}{4}f(2J_1) - \frac{1}{2}f(J_1,)$$

$$B_7 = \frac{1}{4}f(J_s + 2J_1) + \frac{1}{4}f(J_s - 2J_1) - f(J_s + J_1) - f(J_s - J_1) + \frac{3}{2}f(J_s)$$

$$B_8 = \frac{1}{2}f(J_s + J_1) - \frac{1}{2}f(J_s - 2J_1) - f(J_s + J_1) + f(J_s - J_1, \Omega_s) - f(2J_1, \Omega_s) + 2f(J_1)$$

$$C_1 = f(J_2)$$

$$C_2 = -f(J_2) + \frac{1}{2}f(2J_2)$$

$$C_3 = \frac{5}{4}f(J_2) - f(2J_2) + \frac{1}{4}f(3J_2)$$

$$C_4 = -\frac{7}{4}f(J_2) + \frac{7}{4}f(2J_2) - \frac{3}{4}f(3J_2) + \frac{1}{8}f(4J_2)$$

$$C_5 = \frac{21}{8}f(J_2) - 3f(2J_2) + \frac{27}{16}f(3J_2) - \frac{1}{2}f(4J_2) + \frac{1}{16}f(5J_2)$$

$$C_6 = -\frac{33}{8}f(J_2) + \frac{165}{32}f(2J_2) - \frac{55}{16}f(3J_2) + \frac{11}{8}f(4J_2) - \frac{5}{16}f(5J_2) + \frac{1}{32}f(6J_2)$$

$$C_7 = -\frac{3}{4}f(J_2) + \frac{1}{4}f(3J_2)$$

$$C_8 = \frac{3}{4}f(J_2) - \frac{1}{4}f(2J_2) + \frac{1}{4}f(3J_2) + \frac{1}{8}f(4J_2)$$

$$C_9 = -\frac{7}{8}f(J_2) + \frac{1}{2}f(2J_2) + \frac{3}{16}f(3J_2) - \frac{1}{4}f(4J_2) + \frac{1}{16}f(5J_2)$$

$$C_{10} = \frac{9}{8}f(J_2) - \frac{27}{32}f(2J_2) - \frac{1}{16}f(3J_2) + \frac{3}{8}f(4J_2) - \frac{3}{16}f(5J_2) + \frac{1}{32}f(6J_2)$$

$$C_{11} = \frac{5}{8}f(J_2) - \frac{5}{16}f(3J_2) + \frac{1}{16}f(5J_2)$$

$$C_{12} = -\frac{5}{8}f(J_2) + \frac{5}{32}f(2J_2) + \frac{5}{16}f(3J_2) - \frac{1}{8}f(4J_2) - \frac{1}{16}f(5J_2) + \frac{1}{32}f(6J_2)$$

$$D_1 = \frac{1}{4}F_1\left(\frac{3}{2}J_1 + \frac{1}{2}J_2\right) + \frac{1}{4}F_1\left(\frac{3}{2}J_1 - \frac{1}{2}J_2\right) + \frac{1}{4}F_1\left(\frac{1}{2}J_1 + \frac{1}{2}J_2\right) + \frac{1}{4}F_1\left(\frac{1}{2}J_1 - \frac{1}{2}J_2\right)$$

$$D_2 = \frac{1}{4}F_1\left(\frac{3}{2}J_1 + \frac{1}{2}J_2\right) - \frac{1}{4}F_1\left(\frac{3}{2}J_1 - \frac{1}{2}J_2\right) + \frac{3}{4}F_1\left(\frac{1}{2}J_1 + \frac{1}{2}J_2\right) - \frac{3}{4}F_1\left(\frac{1}{2}J_1 - \frac{1}{2}J_2\right)$$

$$D_3 = \frac{1}{16} \cdot \left[F_1\left(J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) + F_1\left(J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) + 3F_1\left(J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) + 3F_1\left(J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) - F_1\left(-J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) - F_1\left(-J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) - 3F_1\left(-J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) - 3F_1\left(-J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) \right]$$

$$D_4 = \frac{1}{32} \cdot \left[F_1\left(2J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) + F_1\left(2J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) + 3F_1\left(2J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) + 3F_1\left(2J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) - F_1\left(-2J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) - F_1\left(-2J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) - 3F_1\left(-2J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) - 3F_1\left(-2J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) - 2F_1\left(J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) - 2F_1\left(J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) - 6F_1\left(J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) - 6F_1\left(J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) + 2F_1\left(-J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) + 2F_1\left(-J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) + 6F_1\left(-J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) + 6F_1\left(-J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) \right]$$

$$D_5 = F_1\left(\frac{3}{2}J_1 + \frac{1}{2}J_2\right) + F_1\left(\frac{3}{2}J_1 - \frac{1}{2}J_2\right) - 3F_1\left(\frac{1}{2}J_1 + \frac{1}{2}J_2\right) - 3F_1\left(\frac{1}{2}J_1 - \frac{1}{2}J_2\right)$$

$$D_6 = F_1\left(\frac{3}{2}J_1 + \frac{1}{2}J_2\right) - F_1\left(\frac{3}{2}J_1 - \frac{1}{2}J_2\right) - F_1\left(\frac{1}{2}J_1 + \frac{1}{2}J_2\right) + F_1\left(\frac{1}{2}J_1 - \frac{1}{2}J_2\right)$$

$$4F_1\left(-J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) - 4F_1\left(-J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) + 12F_1\left(-J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) + \\ 12F_1\left(-J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) + 6F_1\left(\frac{3}{2}J_1 + \frac{1}{2}J_2\right) + 6F_1\left(\frac{3}{2}J_1 - \frac{1}{2}J_2\right) - 18F_1\left(\frac{1}{2}J_1 + \frac{1}{2}J_2\right) - \\ 18F_1\left(\frac{1}{2}J_1 - \frac{1}{2}J_2\right)\Big]$$

$$E_1 = \frac{1}{8}F_2\left(\frac{3}{2}J_1 + \frac{1}{2}J_2\right) + \frac{1}{8}F_2\left(\frac{3}{2}J_1 - \frac{1}{2}J_2\right) + \frac{3}{8}F_2\left(\frac{1}{2}J_1 + \frac{1}{2}J_2\right) + \frac{3}{8}F_2\left(\frac{1}{2}J_1 - \frac{1}{2}J_2\right)$$

$$E_2 = \frac{1}{2}F_2\left(\frac{3}{2}J_1 + \frac{1}{2}J_2\right) + \frac{1}{2}F_2\left(\frac{3}{2}J_1 - \frac{1}{2}J_2\right) - \frac{1}{2}F_2\left(\frac{1}{2}J_1 + \frac{1}{2}J_2\right) - \frac{1}{2}F_2\left(\frac{1}{2}J_1 - \frac{1}{2}J_2\right)$$

$$E_3 = \frac{1}{2}F_2\left(\frac{3}{2}J_1 + \frac{1}{2}J_2\right) - \frac{1}{2}F_2\left(\frac{3}{2}J_1 - \frac{1}{2}J_2\right) + \frac{1}{2}F_2\left(\frac{1}{2}J_1 + \frac{1}{2}J_2\right) - \frac{1}{2}F_2\left(\frac{1}{2}J_1 - \frac{1}{2}J_2\right)$$

$$E_4 = 2F_2\left(\frac{3}{2}J_1 + \frac{1}{2}J_2\right) - 2F_2\left(\frac{3}{2}J_1 - \frac{1}{2}J_2\right) - 6F_2\left(\frac{1}{2}J_1 + \frac{1}{2}J_2\right) + 6F_2\left(\frac{1}{2}J_1 - \frac{1}{2}J_2\right)$$

$$E_5 = \frac{1}{16}\cdot\left[F_2\left(J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) + F_2\left(J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) + 3F_2\left(J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) + 3F_2\left(J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) + F_2\left(-J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) + F_2\left(-J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) + 3F_2\left(-J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) + \right. \\ \left. 3F_2\left(-J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) - 2F_2\left(\frac{3}{2}J_1 + \frac{1}{2}J_2\right) - 2F_2\left(\frac{3}{2}J_1 - \frac{1}{2}J_2\right) - 6F_2\left(\frac{1}{2}J_1 + \frac{1}{2}J_2\right) - 6F_2\left(\frac{1}{2}J_1 - \frac{1}{2}J_2\right)\right]$$

$$E_6 = \frac{1}{32}\cdot\left[F_2\left(2J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) + F_2\left(2J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) + 3F_2\left(2J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) + \right. \\ \left. 3F_2\left(2J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) + F_2\left(-2J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) + F_2\left(-2J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) + \right. \\ \left. 3F_2\left(-2J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) + 3F_2\left(-2J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) - 2F_2\left(\frac{3}{2}J_1 + \frac{1}{2}J_2\right) - \right. \\ \left. 2F_2\left(\frac{3}{2}J_1 - \frac{1}{2}J_2\right) - 6F_2\left(\frac{1}{2}J_1 + \frac{1}{2}J_2\right) - 6F_2\left(\frac{1}{2}J_1 - \frac{1}{2}J_2\right)\right]$$

$$E_7 = \frac{1}{32}\cdot\left[F_2\left(2J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) + F_2\left(2J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) + 3F_2\left(2J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) + \right. \\ \left. 3F_2\left(2J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) + F_2\left(-2J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) + F_2\left(-2J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) + \right. \\ \left. 3F_2\left(-2J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) + 3F_2\left(-2J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) - 4F_2\left(J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) - \right. \\ \left. 4F_2\left(J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) - 12F_2\left(J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) - 12F_2\left(J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) - 4F_2\left(-J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) - \right. \\ \left. 4F_2\left(-J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) - 12F_2\left(-J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) - 12F_2\left(-J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) - \right. \\ \left. 6F_2\left(\frac{3}{2}J_1 + \frac{1}{2}J_2\right) + 6F_2\left(\frac{3}{2}J_1 - \frac{1}{2}J_2\right) + 18F_2\left(\frac{1}{2}J_1 + \frac{1}{2}J_2\right) + 18F_2\left(\frac{1}{2}J_1 - \frac{1}{2}J_2\right)\right]$$

$$E_8 = \frac{1}{8}\cdot\left[F_2\left(J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) + F_2\left(J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) + F_2\left(J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) + F_2\left(J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) - F_2\left(-J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) - F_2\left(-J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) - F_2\left(-J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) - F_2\left(-J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right)\right]$$

$$F_2\left(-J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) - 2F_2\left(\frac{3}{2}J_1 + \frac{1}{2}J_2\right) - 2F_2\left(\frac{3}{2}J_1 - \frac{1}{2}J_2\right) + 2F_2\left(\frac{1}{2}J_1 + \frac{1}{2}J_2\right) + 2F_2\left(\frac{1}{2}J_1 - \frac{1}{2}J_2\right)\Big]$$

$$E_{17} = \frac{1}{8} \cdot \left[F_2\left(J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) - F_2\left(J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) + F_2\left(J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) - F_2\left(J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) + F_2\left(-J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) - F_2\left(-J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) + F_2\left(-J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) - F_2\left(-J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) - 2F_2\left(\frac{3}{2}J_1 + \frac{1}{2}J_2\right) + 2F_2\left(\frac{3}{2}J_1 - \frac{1}{2}J_2\right) - 2F_2\left(\frac{1}{2}J_1 + \frac{1}{2}J_2\right) + 2F_2\left(\frac{1}{2}J_1 - \frac{1}{2}J_2\right) \Big]$$

$$E_{18} = \frac{1}{16} \cdot \left[F_2\left(2J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) + F_2\left(2J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) + F_2\left(2J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) + F_2\left(2J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) - F_2\left(-2J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) - F_2\left(-2J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) - F_2\left(-2J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) - F_2\left(-2J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) - 2F_2\left(J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) - 2F_2\left(J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) - 2F_2\left(J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) - 2F_2\left(J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) + 2F_2\left(-J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) + 2F_2\left(-J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) + 2F_2\left(-J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) + 2F_2\left(-J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) \Big]$$

$$E_{19} = \frac{1}{16} \cdot \left[F_2\left(2J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) - F_2\left(2J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) + 3F_2\left(2J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) - 3F_2\left(2J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) - F_2\left(-2J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) + F_2\left(-2J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) - 3F_2\left(-2J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) + 3F_2\left(-2J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) - 2F_2\left(J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) + 2F_2\left(J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) - 6F_2\left(J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) + 6F_2\left(J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) + 2F_2\left(-J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) - 2F_2\left(-J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) + 6F_2\left(-J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) - 6F_2\left(-J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) \Big]$$

$$E_{20} = \frac{1}{4} \cdot \left[F_2\left(2J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) + F_2\left(2J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) - 3F_2\left(2J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) - 3F_2\left(2J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) - F_2\left(-2J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) - F_2\left(-2J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) + 3F_2\left(-2J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) + 3F_2\left(-2J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) - 2F_2\left(J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) - 2F_2\left(J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) + 6F_2\left(J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) + 6F_2\left(J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) + 2F_2\left(-J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) + 2F_2\left(-J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) - 6F_2\left(-J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) - 6F_2\left(-J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) \Big]$$

$$E_{21} = \frac{1}{4} \cdot \left[F_2\left(2J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) - F_2\left(2J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) - F_2\left(2J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) + F_2\left(2J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) - F_2\left(-2J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) + F_2\left(-2J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) + F_2\left(-2J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) - F_2\left(-2J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) - 2F_2\left(J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) + 2F_2\left(J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) + 2F_2\left(J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) - 2F_2\left(J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) + 2F_2\left(-J + \frac{3}{2}J_1 + \frac{1}{2}J_2\right) - 2F_2\left(-J + \frac{3}{2}J_1 - \frac{1}{2}J_2\right) - 2F_2\left(-J + \frac{1}{2}J_1 + \frac{1}{2}J_2\right) + 2F_2\left(-J + \frac{1}{2}J_1 - \frac{1}{2}J_2\right) \Big]$$

$$E_{22} = \frac{1}{8} \cdot \left[F_2 \left(2J + \frac{3}{2}J_1 + \frac{1}{2}J_2 \right) + F_2 \left(2J + \frac{3}{2}J_1 - \frac{1}{2}J_2 \right) - F_2 \left(2J + \frac{1}{2}J_1 + \frac{1}{2}J_2 \right) - \right. \\ \left. F_2 \left(2J + \frac{1}{2}J_1 - \frac{1}{2}J_2 \right) + F_2 \left(-2J + \frac{3}{2}J_1 + \frac{1}{2}J_2 \right) + F_2 \left(-2J + \frac{3}{2}J_1 - \frac{1}{2}J_2 \right) - F_2 \left(-2J + \right. \right. \\ \left. \left. \frac{1}{2}J_1 + \frac{1}{2}J_2 \right) - F_2 \left(-2J + \frac{1}{2}J_1 - \frac{1}{2}J_2 \right) - 4F_2 \left(J + \frac{3}{2}J_1 + \frac{1}{2}J_2 \right) - 4F_2 \left(J + \frac{3}{2}J_1 - \frac{1}{2}J_2 \right) + \right. \\ \left. 4F_2 \left(J + \frac{1}{2}J_1 + \frac{1}{2}J_2 \right) + 4F_2 \left(J + \frac{1}{2}J_1 - \frac{1}{2}J_2 \right) - 4F_2 \left(-J + \frac{3}{2}J_1 + \frac{1}{2}J_2 \right) - 4F_2 \left(-J + \frac{3}{2}J_1 - \right. \right. \\ \left. \left. \frac{1}{2}J_2 \right) + 4F_2 \left(-J + \frac{1}{2}J_1 + \frac{1}{2}J_2 \right) + 4F_2 \left(-J + \frac{1}{2}J_1 - \frac{1}{2}J_2 \right) + 6F_2 \left(\frac{3}{2}J_1 + \frac{1}{2}J_2 \right) + \right. \\ \left. 6F_2 \left(\frac{3}{2}J_1 - \frac{1}{2}J_2 \right) - 6F_2 \left(\frac{1}{2}J_1 + \frac{1}{2}J_2 \right) - 6F_2 \left(\frac{1}{2}J_1 - \frac{1}{2}J_2 \right) \right]$$

$$E_{23} = \frac{1}{8} \cdot \left[F_2 \left(2J + \frac{3}{2}J_1 + \frac{1}{2}J_2 \right) - F_2 \left(2J + \frac{3}{2}J_1 - \frac{1}{2}J_2 \right) + F_2 \left(2J + \frac{1}{2}J_1 + \frac{1}{2}J_2 \right) - \right. \\ \left. F_2 \left(2J + \frac{1}{2}J_1 - \frac{1}{2}J_2 \right) + F_2 \left(-2J + \frac{3}{2}J_1 + \frac{1}{2}J_2 \right) - F_2 \left(-2J + \frac{3}{2}J_1 - \frac{1}{2}J_2 \right) + F_2 \left(-2J + \right. \right. \\ \left. \left. \frac{1}{2}J_1 + \frac{1}{2}J_2 \right) - F_2 \left(-2J + \frac{1}{2}J_1 - \frac{1}{2}J_2 \right) - 4F_2 \left(J + \frac{3}{2}J_1 + \frac{1}{2}J_2 \right) + 4F_2 \left(J + \frac{3}{2}J_1 - \frac{1}{2}J_2 \right) - \right. \\ \left. 4F_2 \left(J + \frac{1}{2}J_1 + \frac{1}{2}J_2 \right) + 4F_2 \left(J + \frac{1}{2}J_1 - \frac{1}{2}J_2 \right) - 4F_2 \left(-J + \frac{3}{2}J_1 + \frac{1}{2}J_2 \right) + 4F_2 \left(-J + \frac{3}{2}J_1 - \right. \right. \\ \left. \left. \frac{1}{2}J_2 \right) - 4F_2 \left(-J + \frac{1}{2}J_1 + \frac{1}{2}J_2 \right) + 4F_2 \left(-J + \frac{1}{2}J_1 - \frac{1}{2}J_2 \right) + 6F_2 \left(\frac{3}{2}J_1 + \frac{1}{2}J_2 \right) - \right. \\ \left. 6F_2 \left(\frac{3}{2}J_1 - \frac{1}{2}J_2 \right) + 6F_2 \left(\frac{1}{2}J_1 + \frac{1}{2}J_2 \right) - 6F_2 \left(\frac{1}{2}J_1 - \frac{1}{2}J_2 \right) \right]$$

$$E_{24} = \frac{1}{2} \cdot \left[F_2 \left(2J + \frac{3}{2}J_1 + \frac{1}{2}J_2 \right) - F_2 \left(2J + \frac{3}{2}J_1 - \frac{1}{2}J_2 \right) - 3F_2 \left(2J + \frac{1}{2}J_1 + \frac{1}{2}J_2 \right) + \right. \\ \left. 3F_2 \left(2J + \frac{1}{2}J_1 - \frac{1}{2}J_2 \right) + F_2 \left(-2J + \frac{3}{2}J_1 + \frac{1}{2}J_2 \right) - F_2 \left(-2J + \frac{3}{2}J_1 - \frac{1}{2}J_2 \right) - \right. \\ \left. 3F_2 \left(-2J + \frac{1}{2}J_1 + \frac{1}{2}J_2 \right) + 3F_2 \left(-2J + \frac{1}{2}J_1 - \frac{1}{2}J_2 \right) - 4F_2 \left(J + \frac{3}{2}J_1 + \frac{1}{2}J_2 \right) + \right. \\ \left. 4F_2 \left(J + \frac{3}{2}J_1 - \frac{1}{2}J_2 \right) + 12F_2 \left(J + \frac{1}{2}J_1 + \frac{1}{2}J_2 \right) - 12F_2 \left(J + \frac{1}{2}J_1 - \frac{1}{2}J_2 \right) - 4F_2 \left(-J + \right. \right. \\ \left. \left. \frac{3}{2}J_1 + \frac{1}{2}J_2 \right) + 4F_2 \left(-J + \frac{3}{2}J_1 - \frac{1}{2}J_2 \right) + 12F_2 \left(-J + \frac{1}{2}J_1 + \frac{1}{2}J_2 \right) - 12F_2 \left(-J + \frac{1}{2}J_1 - \right. \right. \\ \left. \left. \frac{1}{2}J_2 \right) + 6F_2 \left(\frac{3}{2}J_1 + \frac{1}{2}J_2 \right) - 6F_2 \left(\frac{3}{2}J_1 - \frac{1}{2}J_2 \right) - 18F_2 \left(\frac{1}{2}J_1 + \frac{1}{2}J_2 \right) + 18F_2 \left(\frac{1}{2}J_1 - \frac{1}{2}J_2 \right) \right]$$

$$A = [A_2 + (2A_1 + 2A_3 \cdot q_0) \cdot (2B_2 + 2B_6 \cdot q_0)] \cdot [1 - (2A_1 + 2A_3 \cdot q_0) \cdot (2B_1 + 4B_3 \cdot q_0 + 2B_7 \cdot q_0^2)]^{-1}$$

$$B = [A_2 \cdot (2B_1 + 4B_3 \cdot q_0 + 2B_7 \cdot q_0^2) + 2B_2 + 2B_6 \cdot q_0] \cdot [1 - (2A_1 + 2A_3 \cdot q_0) \cdot (2B_1 + 4B_3 \cdot q_0 + 2B_7 \cdot q_0^2)]^{-1}$$

$$C = 6C_1 + 30C_2 \cdot q_0 + 60C_3 \cdot q_0^2 + 60C_4 \cdot q_0^3 + 30C_5 \cdot q_0^4 + 6C_6 \cdot q_0^5$$

$$D = E \cdot (2A_1 + 2A_3 \cdot q_0) + 2A_3 \cdot q_0 \cdot B + A_4 \cdot B^2$$

$$E = \{2B_6 \cdot q_9 + A_2 \cdot (4B_3 \cdot q_9 + 4B_7 \cdot q_0 \cdot q_9) + 2A_2 \cdot B_5 + A_2^2 \cdot (2B_4 + 2B_8 \cdot q_0) + B \cdot (2A_1 + 2A_3 \cdot q_0) \cdot (2B_5 + 4B_3 \cdot q_9 + 4B_7 \cdot q_0 \cdot q_9 + 4A_2 \cdot B_4 + 4A_2 \cdot B_8 \cdot q_0) + (2B_1 + 4B_3 \cdot q_0 + 2B_7 \cdot q_0^2) \cdot (2A_3 \cdot q_9 \cdot B + A_4 \cdot B^2) + B^2 \cdot (2B_4 + 2B_8 \cdot q_0) \cdot (2A_1 + 2A_3 \cdot q_0)^2\} \cdot \{1 - (2A_1 + 2A_3 \cdot q_0) \cdot (2B_1 + 4B_3 \cdot q_0 + 2B_7 \cdot q_0^2)\}^{-1}$$

$$F = 20C_7 + 60C_8 \cdot q_0 + 60C_9 \cdot q_0^2 + 20C_{10} \cdot q_0^3 + 30C_2 \cdot q_9 + 120C_3 \cdot q_9 \cdot q_0 + 180C_4 \cdot q_9 \cdot q_0^2 + 120C_5 \cdot q_9 \cdot q_0^3 + 30C_6 \cdot q_9 \cdot q_0^4$$

$$\begin{aligned}
q_1 &= \frac{E_2 + 2E_{12} \cdot q_0 + E_{22} \cdot q_0^2}{1 - 2E_5 - 2E_7 \cdot q_0}, & q_2 &= \frac{E_6}{1 - 2E_5 - 2E_7 \cdot q_0} \\
q_3 &= \frac{2E_8 + 2E_{18} \cdot q_0}{1 - 2E_5 - 2E_7 \cdot q_0}, & q_4 &= \frac{4E_8 + 4E_{18} \cdot q_0}{1 - 2E_5 - 2E_7 \cdot q_0} \\
q_5 &= \frac{2E_9 + 2E_{19} \cdot q_0}{1 - 2E_5 - 2E_7 \cdot q_0}, & q_6 &= \frac{2E_2 + 4E_{12} \cdot q_0 + 2E_{22} \cdot q_0^2}{1 - 2E_5 - 2E_7 \cdot q_0} \\
q_7 &= \frac{E_3 + 2E_{13} \cdot q_0 + E_{23} \cdot q_0^2}{1 - 2E_5 - 2E_7 \cdot q_0}, & q_8 &= \frac{2E_3 + 4E_{13} \cdot q_0 + 2E_{23} \cdot q_0^2}{1 - 2E_5 - 2E_7 \cdot q_0} \\
q_9 &= q_1 \cdot B^2 + q_2 + q_3 \cdot A + q_4 \cdot B + q_5 \cdot C + q_6 \cdot A \cdot B + q_7 \cdot A \cdot C + q_8 \cdot B \cdot C
\end{aligned}$$