Magnetic properties of spherical ferri-magnetic core/shells: A Monte Carlo study

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Abstract: In this work, we study the magnetic properties of a spherical ferrimagnetic core/shell, formed with nanoparticles of a spin-1/2 in the core surrounded by spin-1 in the shell layer. An external magnetic field is applied on this system. In addition, we examined the magnetizations as well as the susceptibilities of this system, for specific values of the coupling constants between the spins of the shell-shell Js, the core-shell Jp and core-core Jc. The response of the magnetization to the field is illustrated in the hysteresis loops.

PACS: 73.63.Fg; 77.80.B-; 71.70.Gm; 34.20.Gj.; 81.16.Ta

Introduction:

Nanoparticles, aggregates of a few tens to millions of atoms or molecules, have attracted enormous interest from either basic science or application point of view in the past decades.

From application point of view, highly stable nanoparticles can serve as building blocks for assembly of new materials and for design of nano-devices. Also, size-dependent characteristics open a possibility for tailoring properties of nanoclusters by precisely controlling the formation process.

Among these nanomaterials, core/shells are of considerable interest for both theoretical and experimental studies because of their wide range for potential technological applications, such as magnetic storage devices [1], sensors [2], permanent magnets [3] and medical applications [4]. Indeed, many methods have been used to fabricate core/shells, such as the electrochemical method [5], radiolysis of aqueous solutions [6], hydrogen arc plasma [7] and laser vaporization codeposition [8].

Recently, core/shell nanoclusters have received considerable attention owing to their physical and chemical properties that are strongly dependent on the structure of the core, shell, and their interface. This structure dependence opens possibility for tuning properties by controlling their chemical composition and relative size of the core and shell. The core–shell magnetic nanoclusters are of special interests since the heterogeneous nanostructures offer opportunities for developing devices and cluster assembled materials with new functions for magnetic recording, bio, and medical applications. In fact, superparamagnetic nanoparticles with suitable biocompatible coatings have important implications in biology, biotechnology, and other biomedical disciplines [9-11].

In addition, the physical properties (the core, the shell and the interaction parameters) of these structures can be theoretically described very easily using different methods; many studies have been devoted to investigate the equilibrium

thermal and magnetic properties using the core–shell concept and several types of methods such as mean field theory (MFA) and the effective field theory with correlation (EFT) [12,13].
Moreover, the magnetic properties of the nanostructures have been studied by using Monte Carlo (MC) simulations [14–20].
The aim of this work is to study the magnetic properties of a system composed by a spherical ferrimagnetic nanoparticles of a spin-1/2 in the core spheres which is surrounded by a spin-1 in the shell layer under the influence of an external magnetic field and a crystal field. Indeed, at the interface, there is an antiferromagnetic interaction between core and shell spins.

For this purpose, the outline of the paper is as follows: in Section 2 we briefly present our model. The results and discussion are presented in Section 3, and finally Section 4 contains our conclusions.

II. Theoretical model

We consider a spherical ferrimagnetic core/shell nanoparticle with radius R_N composed of a spin-1/2 in the core with radius $R=R_1$, R_2 ,…, R_{N-1} (N is the number of spheres) which is surrounded by a spin-1 in the shell with a radius R_N.

The Hamiltonian governing the studied system is given by the following terms:

$$H = H_{shell} + H_{core} + H_{\text{int}} + H_h + H_d \quad (1)$$

$$H_{shell} = -J_S \sum_{i,j \in shell} S_k S_l \quad (2)$$

$$H_{core} = -J_C \sum_{i,j \in core} \sigma_i \sigma_j \quad (3)$$

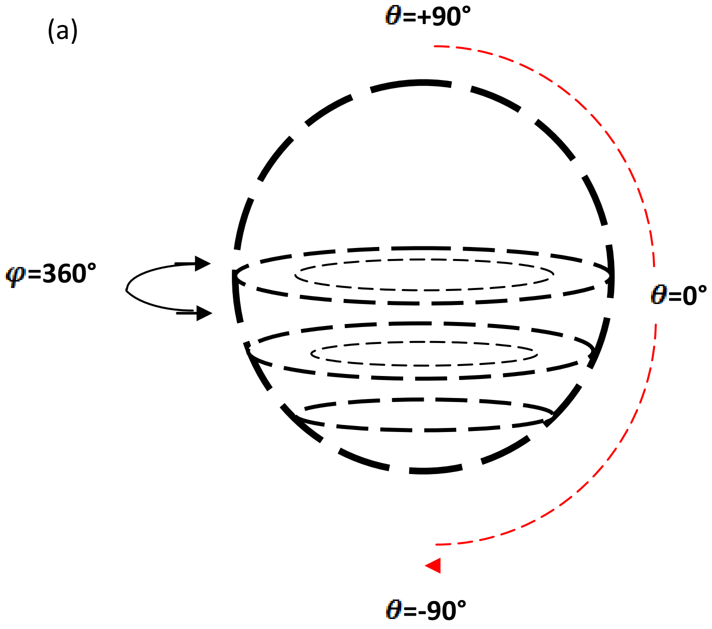
$$H_{\text{int}} = -J_P \sum_{i \in shell, j \in core} S_i \sigma_j \quad (4)$$

$$H_h = -h \sum_{i \in shell+core} (\sigma_i + S_i) \quad (5)$$

$$H_d = -\Delta \sum_{i \in shell} S_i^2 \quad (6)$$

The equation (2) coresponds to the energy interaction of the shell sphere described by the radius $R= R_N$. Where as the equation (3) illustrates the core spheres corresponding to the energy interaction of the spheres with radii $R=R_1$, R_2 ,…, R_{N-1}. The above equation (4) describes the energy interaction between the shell and the core spheres. The term (5) gives the energy interaction under the external magnetic field h. The final equation (6) corresponds to the crystal field energy which is applied only on spins-S.
J_S, J_C and J_P are the exchange interactions between nearest-neighbors magnetic atoms in the shell, core and core-shell interface of the particles between nearest-neighbors spins.
In the above equations, $\sigma = \pm\frac{1}{2}$ and $S=\pm 1,0$ are spin variables belonging to the core and the shell, respectively (see Fig. 1). Each spin σ or S is located with three variables (φ, θ, R), where $R= R_N$ for the shell (spins S) and $R< R_N$ for the core (spins σ) , as it is well illustrated in Figs. 1(a,b). For each site (φ, θ, R) belonging to a sphere of radius R, the spherical angles satisfy the following conditions: $0 \le \varphi \le 360°$ and $-90° \le \theta \le +90°$.

(a)



(b)

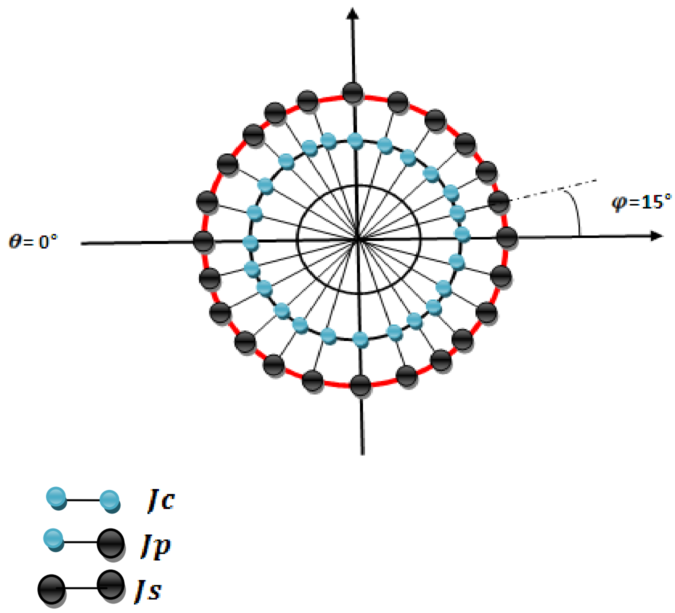


Fig. 1: Schematic representation of a spherical core–shell nanoparticle with a spin-1/2 core and spin-1 shell. The constant coupling between the spins σ (blue atom) and σ is denoted by J_C, between the spins S and S is denoted by J_S (black atom), while J_P denotes the constant coupling between the core and shell.

We applied the Monte Carlo simulations under Metropolis algorithm for standard sampling method to simulate the Hamiltonian given by Eq.(1). The simulations were performed for N radii varying from R_1 , R_2 ,…, R_N (R_N corresponds to the shell sphere). Preliminary results were carried out for several system sizes in order to determine the size effect. Numerical results were performed for the specific sizes: N=3, 5 and 7 spheres.

The flips are accepted or rejected according to a heat-bath algorithm. Starting from different initial conditions, we perform 10^5 Monte Carlo steps (MCS) for each spin configuration, and discarding the first 10^4 generated configurations. We average over many configurations for each initial condition. Our programs calculate the following parameters, namely:

The internal energy per site:

$$E = \frac{1}{V_T} < H > \quad (6)$$

Where, $V_T = V_{core} + V_{shell}$ is the total volume of the core and the shell of the system.

The magnetizations per site:

$$M_{shell} = \frac{1}{V_{shell}} \sum_{i \in shell} S_i \quad (7)$$

$$M_{core} = \frac{1}{V_{core}} \sum_{i \in core} \sigma_i \quad (8)$$

The corresponding total magnetization is:

$$M_{tot} = \frac{M_{shell} + M_{core}}{2} \quad (9)$$

The magnetic susceptibilities are given by:

$$\chi_{shell} = \beta(< M^2_{shell} > - < M_{shell} >^2) \quad (10)$$

$$\chi_{core} = \beta(< M^2_{core} > - < M_{core} >^2) \quad (11)$$

Where $\beta = \frac{1}{k_B T}$, and k_B is the Boltzmann constant. We take $k_B = 1$ in all the following.

IV. Results and discussions

In this section, we study the effect of the antiferromagnetic interface coupling on the compensation temperature of the spherical nanoparticle model with core/shell morphology using the Monte Carlo simulation technique.

From total magnetization M_{tot} profile for various system sizes, we found that with increasing the number of core R_N the compensation temperature decreases which corresponds to the first peak of susceptibility, see Fig2 (a,b,c). But

the critical temperature does not undergo a major change by changing this number of core sphere.

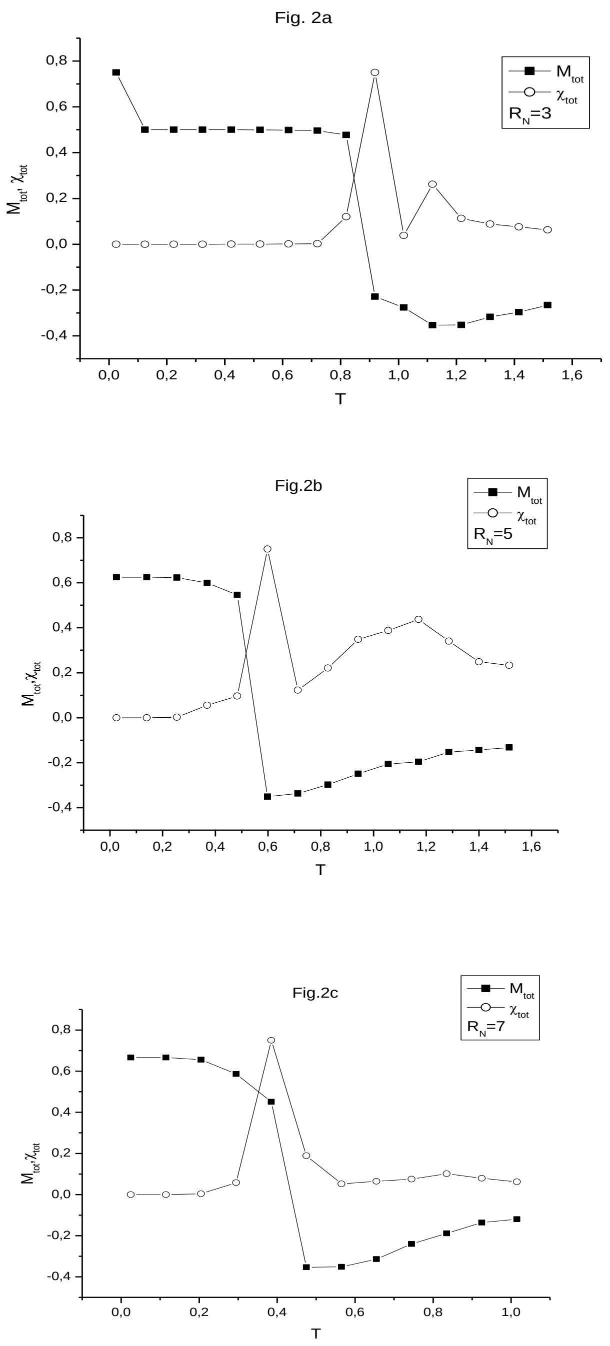


Fig. 2: The variation of total magnetization M_{tot} and the total magnetic susceptibility χ_{tot} as a function of temperature T, with varying the number of sphere shell from R_N= 3 to R_N = 7. (a): R_N =3 and (b): R_N =5 (c) R_N =7.

A great deal of information can be learned about the magnetic properties of a material by studying its hysteresis loop. An example of hysteresis loop is shown in Fig.3. We show the dependence of hysteresis loops on sizes keeping the values of the temperature T=1 K. From these results, we can see that by varying the sizes of core the form of the hysteresis loop changes. It is found that the value of the coercive field corresponds to the lowest value of the number of the core R_N. Also, by increasing the number of the inner sphere of the core, we reach the same value of coercive fields. Indeed, on the remanent magnetization we found that it decreases when the number of the core spheres increases. Therefore, the remanent magnetization and coercive field undergoes modifications.

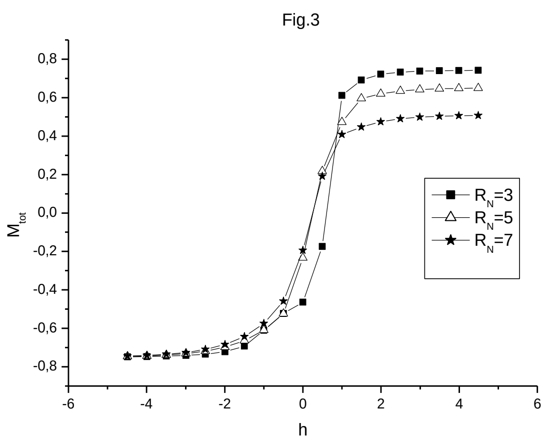


Fig. 3: Magnetization hysteresis loops for the temperature T=1 k, with varying the number of size core from R_N=3 to R_N=7.

In Fig. 4, we presented the magnetization versus the exchange interaction J_P between the core and the shell at a fixed temperature and different sizes. For J_P anti-ferromagnetic, the total magnetization has a value around 0.5 for all size, but by increasing the coupling between core and shell, we get that the effect of this parameter

decreases the magnetization of the system. In addition, we deduce that for ferromagnetic Jp the magnetization decreases slightly and its value depend on the size of the core.

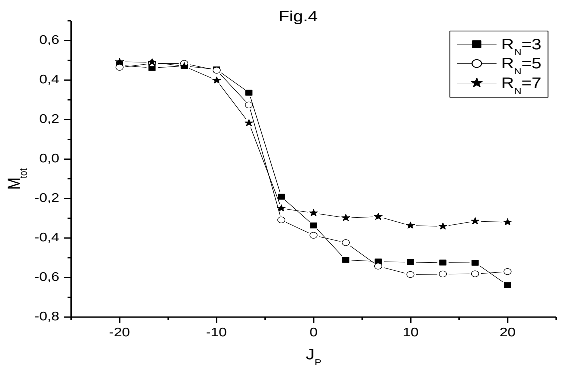


Fig.4: The total magnetization versus the exchange interaction J_P, at different values of R_N=3 to R_N=7, at a fixed temperature value T=1 K.

In order to show the crystal field effect on the spins-shell and spins-core, we plot in Fig. 5, the total magnetizations as a function of crystal field for a fixed value of the temperature T=1 k, with varying the number of the core from R_N=3 to R_N=7.

We see that the magnetizations of different core sizes have almost the same value for a negative crystal field, so that when this field becomes positive, we find the total magnetization of the system depend on the size of the core.

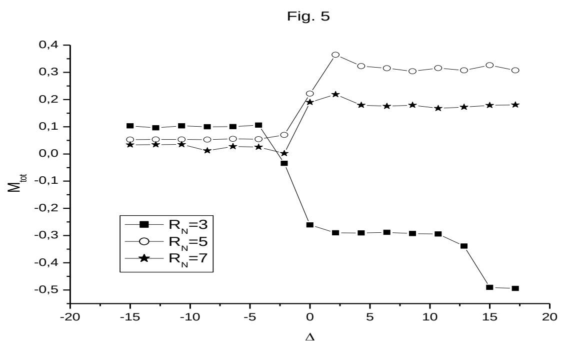


Fig. 5: The variation of total magnetization M_{tot} vs crystal field Δ. For a fixed value of the temperature T=1 k, with varying the number of the core from R_N=3 to R_N=7.

Conclusion

In summary, we have studied the magnetic properties and the compensation behaviors of a spherical ferrimagnetic core/shell nanoparticle on an Ising model, located on a spherical geometry, where we have taken a coupling constants Jc and Js for the core and the shell respectively, and an interface coupling constant JP between the core and the shell with JP<0. An external magnetic field is applied on this system. The system is formed with nanoparticles of a spin-1/2 in the core surrounded by spin-1 in the shell. Using Monte Carlo techniques, we have discussed the influence of the shell and core coupling, the interface coupling and the crystal field on the critical and compensation temperatures. We have shown that total susceptiblity exhibit two sharp peaks, the first one correspond to the compensation temperature and the other one to the critical tempertaure.

Furthermore, the variation of the total magnetization versus crystal field and JP is also obtained for different sizes of shell. Finally, the hysteresis loops are established for different sizes.

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