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Non-equilibrium dynamics of a ferrimagnetic core–shell nanocubic particle

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HIGHLIGHTS

- A ferrimagnetic nanoparticle with spin-1/2 core and spin-1 shell structure is investigated.
- Monte-Carlo simulation with Metropolis algorithm is used.
- The particle is subjected to a time dependent oscillating magnetic field.
- Hamiltonian parameters as well as particle size affect the dynamic nature of the system.
- Sharp transition regions are observed with increasing applied field period.

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ABSTRACT

The non-equilibrium dynamics of a single cubic core–shell ferrimagnetic nanoparticle system under a time dependent oscillating magnetic field is elucidated by making use of a classical Monte Carlo simulation technique with a standard Metropolis algorithm. Many interesting and unusual thermal and magnetic behaviors are observed, for instance, the locations of dynamic phase transition points change significantly depending upon amplitude and period of the external magnetic field as well as other Hamiltonian parameters in related planes. Much effort has also been devoted to the influences of the varying shell thickness on the thermal and magnetic properties of the particle, and outstanding physical findings are reported in order to better understand the dynamic process of the studied nanoparticle system.

1. Introduction

With the reduction of the physical size of a magnetic system to a characteristic length, the surface to volume ratio increases. As a result of this process, the thermal and magnetic properties of the system begin to sensitively depend on the size which is different from those observed in the bulk material. Influences of finite-size originating from the nanometric size of particle and surface effects due to the symmetry breaking of the crystal structure of the particle on the magnetic properties of magnetic nanoparticles have provided a conspicuous and productive field for the interaction between theoretical works [1] and technological [2–4] as well as biomedical applications [5–8]. On the theoretical picture, equilibrium properties of a great number of nanoparticle systems have been studied by employing some of the well defined physical methods such as molecular field approximation (MFA) [9–12], effective field theory (EFT) [12–14], Monte Carlo (MC) simulations [9,10,15–20] and Green function formalism [21,22]. From the experimental point of view, it is possible to mention that due to the recent developments in chemical synthesis techniques scientists are able to produce various types of controllable nanoscaled materials

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such as nanowires, nanotubes, nanorods, nanocubes as well as other more complex shapes [23–32] and they have many applications in different types of nanotechnology areas [33,34]. For example in Ref. [30], a closed-form theory for the investigation of smallest diameter of metallic nanorods has been formulated by benefiting from physical vapor deposition. Moreover, the results obtained from the theory have been verified by making use of lattice kinetic Monte-Carlo simulation technique.

The statistical mechanics of non-equilibrium systems is a less developed and understood field of study than that for equilibrium systems. It is a fact that a magnetically interacting system under the influence of a time dependent oscillating magnetic field exhibits two important striking phenomena: Non-equilibrium phase transitions and dynamic hysteresis behavior. Nowadays, these types of non-equilibrium systems are in the center of scientists' attention because they have exotic, unusual and interesting behaviors. For example, the universality classes of the Ising model and its variations under a time dependent driving field are different from its equilibrium counterparts [35–37]. It is possible to emphasize that non-equilibrium phase transitions originate due to a competition between time scales of the relaxation time of the system and oscillating period of the external applied field. To our knowledge, for the high temperatures and high amplitudes of the periodically varying magnetic field, the system exists in a dynamically disordered phase where the time dependent magnetization is able to follow the external applied magnetic field with some delay whereas this is not the case for low temperatures and small magnetic field amplitudes. The physical mechanism described above points out the existence a dynamic phase transition [35,38,39]. Apart from the investigation of dynamic properties of infinite size systems, there exists an another research area attracting attention both experimentally and theoretically. This area is the examination and determination of the physical and magnetic properties of nanoparticles under the influence of an alternating magnetic field. At this point, it is beneficial to talk briefly about their well known features. For example, when magnetic nanoparticles are subjected to a periodically varying time-dependent magnetic field, the particles may not respond to the external magnetic field instantaneously, which causes interesting behaviors due to the competing time scales of the relaxation behavior of the particles and periodic external magnetic field. The aforementioned situations may give rise to the existence of heating effects related to losses during the magnetization reversal process of the particles. By means of the above discussed properties, the suspensions including suitable magnetic nanoparticles have received intense focus for cancer treatment with magnetic hyperthermia. It has been reported by the previously published studies in the literature that the efficiencies of nanoparticles leading to a heating process sensitively depend on the frequency and amplitude of the external applied field as well as the other particle features [40,41]. In this regard, the experimental and theoretical works concerning the physical investigation of nanoparticles under a time dependent magnetic field have a particularly important role in creating a better understanding of the mechanism underlying these types of systems.

On the other hand, we learned from theoretical studies mentioned below that clarification of thermal and magnetic properties of different shaped magnetic nanoparticle systems under the time dependent oscillating forcing field is possible by making use of well defined non-equilibrium statistical mechanical tools. For example, in Refs. [42,43], thermal variations of time averaged magnetizations, dynamic correlations between time dependent magnetic field and magnetization and hysteresis loop areas of cylindrical Ising nanowire and nanotube systems have been elucidated by benefiting from a Glauber type stochastic process [44], and it is reported that depending on Hamiltonian parameters, the considered systems exhibit different types of magnetization profiles, according to the Néel theory of ferrimagnetism [45,46]. Moreover, a comprehensive MC simulation study with standard Metropolis algorithm has been carried out to determine the dynamic phase transitions, hysteretic as well as finite size properties of a single ferrimagnetic nanocubic system with a core–shell structure, and a number of interesting and unusual behaviors are observed such as in the presence of ultrafast switching fields, the particle may exhibit a dynamic phase transition from paramagnetic to a dynamically ordered phase with increasing ferromagnetic shell thickness [47]. Very recently, a spherical core–shell nanoparticle system with a spin-3/2 core surrounded by a spin-1 shell layer with antiferromagnetic interface coupling is exposed to a sinusoidal magnetic field and it is found that dynamic phase boundaries strongly depend on the Hamiltonian parameters such as for the high amplitude and period values of the external field, the phase transition temperature sharply changes whereas it tends to slowly alter as the reduced magnitude of interlayer parameter increases. Moreover, it is observed that the magnetization curves of the particle have been found to obey P-type, N-type and Q-type classification schemes under certain conditions [48].

It is clear from the previously published works discussed above that equilibrium phase transition properties of different types of nanoparticle systems are clearly indicated, whereas non-equilibrium counterparts deserve a particular attention. From this point of view, a cubic nanoparticle composed of a spin-1/2 ferromagnetic core which is surrounded by a spin-1 ferromagnetic shell layer under the influence of a time dependent driving magnetic field is selected to determine the influences of the internal and external parameters as well as particle size on the dynamic phase transition properties of the cubic core–shell nanoparticle system. The main motivation of the present paper is to attempt to clarify the physical facts underlying these points. 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.

2. Formulation

A single cubic ferrimagnetic nanoparticle made of a spin-1/2 ferromagnetic core which is surrounded by a spin-1 ferromagnetic shell layer is considered. At the interface, an antiferromagnetic interaction between core and shell spins is defined. The particle is subjected to a time varying sinusoidal magnetic field. The Hamiltonian describing our model of the