

A Study of Magnetic Behaviour for Nanoparticles

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Abstract In this paper we will analyse the ferromagnetism in nanoparticles. We will try to explain why materials that do not exhibit magnetism at large scales, exhibit magnetism when nanoparticles of the same material are formed. This occurs because when the particle size is reduced, only one domain can form in one nanoparticle. These nanomaterials then exhibit magnetism at a large scale.

Keywords: nanoparticle, quantum confinement, ferromagnetism, lagrangian

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1. Introduction

Magnetism, the phenomenon by which materials exhibiting this property attract or repel effectively or exert influence on other materials, has a very ancient history which has been familiar to man since 800 B. C. [1,2]. In the whole periodic table, among the transition metals there are iron (Fe), cobalt (Co), nickel (Ni), their alloys, ferrites etc [3] and some of the rare earth metals such as gadolinium (Gd) which exhibit the property of ferromagnetism [2]. This property is not due to their structures because each have different structures and these structures are similar to those of non-ferromagnetic metals as well. Magnetic materials like iron, cobalt, nickel etc do all have partially filled or nearly full d or f bands [3] but are less diffused i.e narrow [2]. As compared to 4s and 4p orbitals the 3d orbitals are less diffused i.e concentrated nearer to atomic nuclei. For example, if we consider a crystal of N-atoms, 5N levels must be accommodated as there are five 3d orbitals [2]. By virtue of more electrons and a narrow band the density of states in average must be much higher than in other bands and in particular the density of states near the Fermi-level is high. In such a situation, it is energetically favourable to have large number of unpaired electrons at the cost of populating higher energy levels making these elements rich in unpaired electrons. However, the understanding of the underlying principles and mechanisms that explain magnetic phenomenon has eluded scientists, until relatively recent times, because of their complex and subtle nature [1]. According to domain theory of ferromagnetism, every ferromagnetic material is composed of small volume regions called domains below a certain temperature T_c called curie temperature [1].

Within each domain all magnetic moments are aligned in the same direction and each domain is magnetised to its saturation magnetisation. According to Weiss molecular field theory, the spontaneous magnetisation in a ferromagnetic material arises because of co-operation between atomic dipoles within a single domain [4]. The internal molecular field H_i , which is produced due to interaction between atomic dipoles, tend to align spins parallel to the field and is given as $H_i = \lambda M$, where λ is called Weiss constant. Thus $H_{eff} = H + H_i = H + \lambda M$, called effective field, makes Curie law hold for ferromagnetic materials. Now, $\chi = M/H_{eff} = C/T$, where C is the Curie constant of the material. Using $H_{eff} = H + H_i = H + \lambda M$, we get $\chi = C/(T - \lambda C)$. When $T = \lambda C$, χ diverges, which means λC is the transition temperature. Thus, $\chi = C/(T - T_c)$ and this type of behavior of susceptibility is exhibited by the ferromagnetic materials. But at $T_c = 1000K$, $H_i \approx 10^7 G$ or $10^3 T$, which is much larger than 0.1T due to simple dipole - dipole interaction, and hence these dipole - dipole interactions cannot be the origin of the molecular field. In a more microscopic treatment, the ferromagnetism occurs due to the strong electron-electron interactions [3]. As per the Pauli's exclusion principle no two electrons can accommodate the same quantum state, with the result the electrons with parallel spins avoid each other spatially giving rise to exchange interactions. These exchange interactions are responsible for the magnetic phenomena according to quantum theory of magnetism.

At the nanoscale, we deal with nanostructured systems, or nanosystems or nanomaterials which include materials systems with particle size within 1-100 nm [5]. In an

extended way, nanomaterials include structures with at least one dimension below 100 nm and second dimension below $1\mu m$ [6]. As compared to their bulk counterparts, nanomaterials display unique and unusual properties due to emergence of quantum effects which mainly emerge due to reduction in one or more dimensions to the nanometer scale [3]. Moreover, it is because of such quantum effects that the ferromagnetic state is induced in nanomaterials. Experimentally, the magnetic properties of nanoscale magnetic semiconductors may be enhanced by several methods and in particular by using magnetic atoms as dopants, such as manganese (Mn) or Vanadium (V), in common semiconductor compounds [7]. Carbon coated nanoparticles iron (Fe), nickel (Ni) and cobalt (Co) having dimensions upto 100 nm, produced by PCVD (pressure chemical vapour deposition) are ferromagnetic upto a temperature of 400 K and are promising candidates for biomedicine applications [3].

2. Ferromagnetism

As the nanoparticle has all the 3-dimensions in nanometer range, it may be associated with a single domain [3]. Within a single domain, a local magnetic moment sits on each site, aligned parallel to each other, which is denoted by a unit vector \vec{n}_j , where j labels the site [8]. As far as magnetic moments, within a single domain, on neighbouring sites are concerned, they have the tendency to point in the same direction. In other words, the energy is

$$\mathcal{H} = J \sum_{\langle i,j \rangle} \vec{n}_i \cdot \vec{n}_j \quad (1)$$

where i, j label neighboring sites and \vec{n}_j is a unit vector denoting a local magnetic moment. For ferromagnetic nature $J < 0$.

In an attractive and a more microscopic treatment, we would take with a Hamiltonian (such as Hubbard Hamiltonian) describing the hopping of magnetic moments and interaction between them. In nanomaterials, the reduction in one or more dimensions results in the decrease of number of nearest neighbours to an atom (i.e, reduction in co-ordination number) thereby reducing the hopping tendency of magnetic moments from one site to another within a domain [3]. The consequences of all this are, the kinetic energy (bandwidth) is reduced and enhancement in the ratio of coulomb interactions and bandwidth, which leads to the occurrence of magnetism in materials with reduced dimensions. By making some suitable and approximate mean field the classical variable \vec{n}_j [8] would then emerge as a unit vector pointing in the direction of $c_j^\dagger \vec{\sigma} c_j$ with c_j^\dagger and c_j the electron creation and annihilation operator, respectively.

2.1. First Verses Second Order in Time

Here, in the light of σ model, we would like to derive the low energy description [8]. A somewhat subtle issue here is that what kinetic energy we should add to \mathcal{H} to form the Lagrangian. The possibility of adding one time derivative is ruled out here because for a unit vector \vec{n} we

have $\vec{n} \cdot d\vec{n}/dt = d(\vec{n} \cdot \vec{n})/dt = 0$. With two time derivatives however, we can form $(d\vec{n}/dt) \cdot (d\vec{n}/dt)$ and so

$$L_{wrong} = \frac{1}{2g^2} \sum_j \frac{\partial \vec{n}_j}{\partial t} \cdot \frac{\partial \vec{n}_j}{\partial t} - J \sum_{\langle i,j \rangle} \vec{n}_i \cdot \vec{n}_j \quad (2)$$

Using the field theory in continuous limit, we would arrive at the Lagrangian density

$$\mathcal{L} = \frac{1}{2g^2} \left(\frac{\partial \vec{n}}{\partial t} \cdot \frac{\partial \vec{n}}{\partial t} - c_s^2 \sum_l \frac{\partial \vec{n}}{\partial x^l} \cdot \frac{\partial \vec{n}}{\partial x^l} \right) \quad (3)$$

with the constraint $[\vec{n}(x,t)]^2$. This is an example of a nonlinear σ model. The constraint c_s is spin wave velocity, which is derived in terms of microscopic variable J as is clear by writing down the equation of motion.

$$\left(\partial^2 / \partial t^2 \right) \vec{n} - c_s^2 \nabla^2 \vec{n} = 0 \quad (4)$$

But, careful examination of the above equation reveals that there is something wrong with the equation. This argument is backed by quantum mechanics since the dynamics of a spin variable \vec{S} is first order in time. This is also supported by solid state physics where-in the dispersion relation of spin wave has non-relativistic form $\omega \propto K^2$ and nor the relativistic form $\omega^2 \propto K^2$ as implied by the above equation (3). The resolution of this apparent paradox is based on the Pauli-Hopf identity. For a unit vector \vec{n} we can always write $\vec{n} = z^\dagger \vec{\sigma} z$, where

$$z = \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}$$

z consists of two complex numbers such that

$$z^\dagger z = z_1^\dagger z_1 + z_2^\dagger z_2 = 1 \quad (5)$$

So the corrected version of (2) is

$$L_{correct} = t \sum_j z_j^\dagger \frac{\partial z_j}{\partial t} + \frac{1}{2g^2} \sum_j \frac{\partial \vec{n}_j}{\partial t} \cdot \frac{\partial \vec{n}_j}{\partial t} - J \sum_{\langle i,j \rangle} \vec{n}_i \cdot \vec{n}_j \quad (6)$$

The added term is known as the Berry's phase term and has a deep topological significance. The above equation of motion can be derived using the identity

$$\int dt \delta \left(z_j^\dagger \frac{\partial z_j}{\partial t} \right) = \frac{1}{2} \int dt \delta \vec{n}_j \cdot \left(\vec{n}_j \times \frac{\partial \vec{n}_j}{\partial t} \right) \quad (7)$$

2.2. Low Energy Modes in the Ferromagnet

As we know in the ground state, the magnetic moments in a single domain point in the same direction, which can be chosen as the z-direction [8]. By expanding the equation of motion in small fluctuations around this ground state $\vec{n}_j = \hat{e}_z + \delta \vec{n}_j$, where \hat{e}_z is the appropriate unit vector and after Fourier transforming, we arrive at the equation

$$\begin{pmatrix} \frac{-\omega^2}{g} + h(k) & -\frac{1}{2}t \\ \frac{1}{2}t & \frac{-\omega^2}{g} + h(k) \end{pmatrix} \begin{pmatrix} \delta n_x(k) \\ \delta n_y(k) \end{pmatrix} = 0$$

which links the two components of $\delta n_x(k)$ and $\delta n_y(k)$.

From the condition $\vec{n}_j \cdot \vec{n}_j = 1$, it is clear that $\delta z(k) = 0$.

Here a is the spacing between the adjacent nanoparticles and

$$h(k) \equiv 4J \left[2 - \cos(k_x a) - \cos(k_y a) \right] \approx 2Ja^2 k^2 \quad (8)$$

for small values of k . The treatment discussed here is for two dimensions. At low frequencies, the Berry's term ω denotes the new term, which can be safely ignored. By setting the determinant of the matrix equal to zero, we arrive at the correct dispersion relation $\omega \propto k^2$ for a single domain of a nanoparticle.

3. Conclusion

In this paper we have analysed ferromagnetism in nanoparticles, which has created enormous interest due to its fruitful applications especially in biomedicine, in the light of quantum field theory. It would be of worth to analyse this phenomena using different techniques of QFT. Further, it would be interesting to analyse another

remarkable phenomena "super paramagnetism" in the light of this theory.

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