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Quantum spin tunneling of magnetization in small ferromagnetic particles

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ABSTRACT

An approach is presented that can also account for the description of small ferromagnetic particle magnetization tunneling. An estimate of the saturation value of an external applied magnetic field along the easy axis is obtained. An analytic expression for the tunneling factor in the absence of an external magnetic field is deduced from the present approach that also allows one to obtain the crossover temperature characterizing the regime where tunneling is dominated by quantum effects.

1. Introduction

Single-domain magnetic particles constitute a scenario in which macroscopic quantum tunneling can be studied. In such systems of mesoscopic size the electronic spins can form an aligned magnetic state that can be oriented in several directions. Quantum mechanics can then be called upon to estimate the tunneling probability that may occur, associated with the possibility of a change of the magnetization from one direction to another. The existence of an energy barrier to be tunneled that do not completely disappear even with a decrease in the temperature towards absolute zero has therefore been suggested and several attempts have been presented in order to estimate the rate of tunneling in these cases [1–4]. In some approaches an adapted version of the WKB is proposed, while, from another perspective, other approaches make use of Feynman's path integral with $su(2)$ coherent states from which the instanton method follows to treat this same quantum problem for a single spin in predicting the energy level splitting.

In general, those approaches start with a Hamiltonian that is associated with a model of the physical system and some considerations are presented in order to get a pair of complementary operators which should characterize the degree of freedom. To this end, the spin system which is actually characterized by a finite-dimensional state space, is converted into a continuous one by means of a transformation which leads to a pair of canonical operators satisfying a new commutation relation which is now dependent on the particle spin quantum number [5]. It is to be observed that this construction is valid for large spin values and that corrections of quantum character must be introduced for small/medium values.

In the present paper we intend to apply a new quantum description originally proposed to treat magnetic molecules of low and intermediate spins [6,7] to ferromagnetic particles. We will show that it can be used in such a way that the energy level splitting in ferromagnetic particles can also be obtained in a direct and simple way. In fact, the formalism also embodies the possibility of describing high spin systems because it is given in terms of expressions that are not *a priori*

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restricted to a particular range of the spin value. As shown elsewhere [6], the proposed approach gives a reliable description for physical systems with spin $S \geq 5$. It does not require new commutation relations connecting pairs of new canonical operators specially constructed for high spin systems; in this way, the usual commutation relations associated with the angular momentum operators is the basic algebraic tool for treating systems of any spin value ($S \geq 5$). Therefore, given the phenomenological Hamiltonian, the ferromagnetic particle properties can be described within this formalism by just taking the limit $S \gg 1$ in the associated corresponding expressions.

The paper is organized as follows. In Section 2 we use the formalism [6] to discuss a phenomenological Hamiltonian associated with a ferromagnetic particle submitted to an external magnetic field. In Section 3, selected properties of ferromagnetic particles will be discussed, namely the energy spectrum and the saturation magnetic field. Also, analytic expressions for the lowest doublet energy gap and the crossover temperature are obtained. Section 4 is devoted to the conclusions.

2. Aspects of the formalism

Before directly treating the magnetic moment tunneling in ferromagnetic particles, let us first prepare the stage for the main aspects of the theoretical background used for that purpose. To this end, the starting point of the proposed approach is the introduction of a quantum phenomenological Hamiltonian describing the spin system, for instance,

$$\mathcal{H} = \mathcal{H}\left(S_z, S_x, S_y, S_z^2, S_x^2, S_y^2\right) \tag{1}$$

written in terms of angular momentum operators obeying the standard commutation relations, and that reflects the internal symmetries of the system. It may also contain terms taking into account external applied magnetic fields. Furthermore, the degree of freedom that undergoes tunneling is considered a particular collective manifestation of the system, and it is assumed to be the only relevant one. At the same time, the temperature of the system is assumed so conveniently low that possible related thermally assisted processes are not taken into account so that only quantum effects are considered.

The next step consists in getting a new Hamiltonian that is an approximate version of Eq. (1). This new Hamiltonian is obtained through a series of transformations performed on the matrix generated by calculating the expectation values of Eq. (1) with the $su(2)$ coherent states $|j, z\rangle$, where z is a complex variable and $j = S$ characterizes the angular momentum state multiplet [8]. The Hamiltonian in the overcomplete spin coherent states representation is then given by

$$\langle j, z'|\mathcal{H}|j, z\rangle = K\left(z', z\right), \tag{2}$$

the also known generator coordinate energy kernel [9]; it embodies all the quantum information related to the system we want to study. The procedure of extracting a new Hamiltonian – written now in terms of an angle variable – from Eq. (2) has been already shown elsewhere and will not be repeated here [6,10]. In fact, as it was proved there, the variational generator coordinate method can in this case be used to rewrite the Hamiltonian from which we start in an exact and discrete representation which can then be conveniently treated in order to give an approximate Hamiltonian in the polar angle representation. It is important to point that the Hamiltonian we obtain is in fact an approximate one, but we have also shown, by studying the Lipkin model [11], that it is already a reliable Hamiltonian for spin systems with $S \gtrsim 5$ [6]. Furthermore, since this approach is based on quantum grounds from the beginning, it does not need to go through any quantization process. Also, it is not necessary to convert the discrete spin system into a continuous one as it is usually done [5], at the same time that the quantum character of the angle-angular momentum pair is properly taken into account.

Based on these considerations, we can now apply the formalism for treating the spin tunneling in ferromagnetic particles. In this case, since sufficiently small ferromagnetic particles consist of a single magnetic domain [12], the magnetic moment will be taken as the relevant spin operator. Furthermore, we make the assumption that the magnetic moment can be considered the tunneling degree of freedom; this assumption can be made in treating the magnetic moment of a small ferromagnetic particle because of the dominance of the exchange interaction which tends to inhibit the effects of the individual spins of the ferromagnetic particle.

We start from a model Hamiltonian describing the ferromagnetic particle [3]

$$\mathcal{H} = -K_1 S_z^2 + K_2 S_y^2 + K_3 H_z S_z. \tag{3}$$

The parameters $K_1 > 0$ and $K_2 > 0$ are the easy-axis (z-axis) and transverse anisotropies respectively, and K_3 is the constant associated with the interaction between the magnetic moment and an external magnetic field pointing along the z direction. Putting this Hamiltonian in a form that emphasizes the creation and annihilation operators we get

$$\mathcal{H} = AS_z^2 + B\left(S_+^2 + S_-^2\right) + CS^2 + K_3 H_z S_z, \tag{4}$$

where $A = -(K_1 + K_2/2)$, $B = -K_2/4$, and $C = K_2/2$. From a formal point of view, it is interesting to see that this Hamiltonian is akin to that one suggested to describe the Fe_8 magnetic cluster (also with an external magnetic field) and that has been treated elsewhere [6,7].

Now, carrying out all the steps of the approach as mentioned before, we obtain the approximate Hamiltonian in the angle representation, namely

$$H(\theta) = -\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}\theta}\frac{1}{M(\theta)}\frac{\mathrm{d}}{\mathrm{d}\theta} + V(\theta) \tag{5}$$