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The transverse spin-$\frac{1}{2}$ Ising order-disorder superlattice

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Abstract

We apply the Ising model in a transverse field to analyse the properties of $KH_2PO_4/KD_2H_2PO_4$ superlattice using the effective field theory with a probability distribution technique. The dielectric-susceptibility and the macroscopic pyroelectric coefficient are calculated for possible comparison with experimental data. We show for thick layer superlattices, two peaks in the mean dielectric susceptibility and pyroelectric coefficient, as they had two phase transitions, whereas thin-layer superlattices, show one-peak behavior.

Keywords: Ferroelectric; Dielectric response; Phase transitions

1. Introduction

The dependence of ferroelectric behavior on the size and the film thickness effects has been investigated theoretically [1–3] and experimentally [4,5] for a long time. In recent years, the interest in size effects on ferroelectricity was inspired by problems in microelectronics for instance by using materials in nonvolatile memory devices. In addition, recent development of ferroelectric films or superlattices has made them to a subject of practical relevance.

From the theoretical point of view, the Landau–Devonshire theory of ferroelectric phase transitions has been extended for the description of thin films [6–8], and ferroelectric superlattices [9–13], which are of increasing importance. One problem with this approach is that it is not clear how to account for the coupling between layers within a continuum theory. Approaches based on the Ising model in a transverse field [14,15] have the advantage that this coupling is automatically described by an inter-layer exchange coupling. In the last decades, there has been an interesting number of works dealing with the critical behavior of quantum spin systems. The transverse Ising model is the simplest quantum system and has been introduced to explain the phase transition of hydrogen-bonded ferroelectrics such as KH_2PO_4 and other systems (a more detailed application has been reviewed in Ref. [16]) for instance the order-disorder phenomenon with tunnelling effects.

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Since then, it has been successfully applied to several physical systems, such as a cooperative Jahn–Teller system [17] (like $DyVO_4$ and $TbVO_4$), ordering in rare earth (RE) compounds with a crystal-field ground state [18], and also to some real magnetic materials with strong uniaxial anisotropy in a transverse field [19].

Ferroelectrics with the basic KH_2PO_4 crystal structure have attracted an enormous amount of interest over several decades and recently they have been used as common examples of order-disorder ferroelectrics [20]. From an experimental standpoint the reasons are practical, large single crystals can be grown easily from water solution and they are in general of high optical quality. As a result they yield useful technological devices such as high-speed electro-optic modulators. Theoretically, the occurrence of ferroelectricity in these materials is associated in a large degree with proton tunelling, but a strong coupling to the hear [21]. A KH_2PO_4/KD_2PO_4 (KDP/KD^*P) superlattice is a particularly simple example because the transverse field is nearly the same in both constituents and only the exchange interaction changes significantly at the interface. Our aim in this paper is to study the dielectric and pyroelectric properties of a $(KDP)_{L_A}/(KD^*P)_{L_B}$ using the transverse spin-$\frac{1}{2}$ Ising superlattice within the framework of the effective field theory with a probability distribution technique [22] that accounts for the self-spin correlations functions. This technique is believed to give more quantitatively exact results than the standard mean field approximation and it has the same qualitatively behavior as it [22]. In Section 2, we give the equations that determine the polarizations and the critical temperature of the superlattice as functions of exchange interactions, transverse field and superlattice thickness. The dielectric susceptibility and the pyroelectric coefficient are discussed in Section 3, and a brief conclusion is given in Section 4. Our results are in good agreement with those obtained recently by Wang et al. [23].

2. Model and formalism

We consider a superlattice consisting of two different ferromagnetic materials KDP and KD^*P stacked alternately. For simplicity, we restrict our attention to the case of the simple cubic structure. The periodic condition suggests that we only have to consider one unit cell. A model of $(KDP)_3/(KD^*P)_3$ is depicted in Fig. 1. The exchange coupling between the nearest-neighbor spins in KDP (KD^*P) is denoted by J_A (J_B), while the transverse field is expressed by Ω_i. Here, we consider the interface to be composed of two layers (L_A and L_A+1). J_{AB} stands for the exchange coupling between the nearest-neighbor spins across the interface. The number of atomic layers in the KDP (KD^*P) material is L_A (L_B) and the thickness of the cell is $L = L_A + L_B$. The Hamiltonian of this system is given by

$$H = -\sum_{(i,j)} J_{ij}\sigma_i^z\sigma_j^z - \sum_i \Omega_i\sigma_i^x, \tag{1}$$

where σ_{iz} and σ_{ix} denote the z and x components of a quantum spin $\vec{\sigma}_i$ of magnitude $\sigma = \frac{1}{2}$ at site i. The first sum runs over all nearest-neighbor pairs, the second sum is taken over the spins and J_{ij} stands for one of the three coupling (J_A, J_B, J_{AB}) depending on the location of the spin pairs. Using the effective field theory [22], the nth layer longitudinal and transverse polarizations of the superlattice are derived in the same manner as for the transverse spin-$\frac{1}{2}$ Ising superlattice [24] and they are given by

$$\begin{aligned} p_{n\alpha} = 2^{-N-2N_0} \sum_{\mu=0}^{N}\sum_{\mu_1=0}^{N_0}\sum_{\mu_2=0}^{N_0} \Big\{ & C_\mu^N C_{\mu_1}^{N_0} C_{\mu_2}^{N_0} (1-2p_{nz})^{\mu}(1+2p_{nz})^{N-\mu} \\ & \times(1-2p_{n-1,z})^{\mu_1}(1+2p_{n-1,z})^{N_0-\mu_1}(1-2p_{n+1,z})^{\mu_2}(1+2p_{n+1,z})^{N_0-\mu_2} \\ & \times f_\alpha\left(\frac{1}{2}[J_{n,n}(N-2\mu) + J_{n,n-1}(N_0-2\mu_1) + J_{n,n+1}(N_0-2\mu_2)], \Omega_n\right)\Big\}, \end{aligned} \tag{2}$$

where

$$f_z(y,\Omega_n) = \frac{1}{2}\frac{y}{(y^2+\Omega_n^2)^{1/2}}\tanh\left[\frac{1}{2}\beta(y^2+\Omega_n^2)^{1/2}\right] \tag{3}$$