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Domain-wall profile in the presence of anisotropic exchange interactions: Effective on-site anisotropy

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Starting from a *D*-dimensional *XXZ* ferromagnetic Heisenberg model in an hypercubic lattice, it is demonstrated that the anisotropy in the exchange coupling constant leads to a *D*-dependent effective on-site anisotropy interaction often ignored for $D>1$. As a result the effective width of the wall depends on the dimensionality of the system. It is shown that the effective one-dimensional Hamiltonian is not the one-dimensional *XXZ* version as assumed in previous theoretical work. We derive a new expression for the wall profile that generalizes the standard Landau-Lifshitz form. Our results are found to be in very good agreement with earlier numerical work using the Monte Carlo method. Preceding theories concerning the domain wall contribution to magnetoresistance have considered the role of *D* only through the modification of the density of states in the electronic band structure. This Brief Report reveals that the wall profile itself contains an additional *D* dependence for the case of anisotropic exchange interactions.

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The competition between exchange and anisotropy energies stabilizes the ground state of ferromagnetic systems as a set of domains with different magnetizations.[1] In the region between the domains the magnetization smoothly changes in a way to continuously connect the different sectors. This configuration, known as a domain wall (DW), is relevant to understanding the transport properties[2–4] and the response of such systems to external fields.[5] However, despite the fact that much is known about the magnetic structure of bulk materials,[6] a framework to deal with the most general situation is not available.[7] In some specific situations the theoretical limitations to solve the general problem can be handled, assuming that the exchange interaction is *isotropic* while the anisotropy in the system, in general, can be described by an *on-site*, also called single-spin, interaction. With these assumptions, and using a variational approach, Landau and Lifshitz[8] obtained the exact form of a Bloch wall. They found the profile of the wall to be described by the expression $\cos\,\theta(x)=-\tanh(x/\lambda)$, where $\theta(x)$ is the polar angle of a classical spin vector at position x and λ is half the effective DW width. This kind of one-dimensional distribution of the magnetic moments is always appropriate if the surface effects can be neglected. Under this assumption, a system in any dimension effectively behaves as one dimensional. This simplified model is in very good agreement with the experimental results in a wide variety of investigated materials[9] where the anisotropy mainly comes from the so-called crystalline field. On the other hand, the formation of DWs in uniaxial ferromagnets with two-spin exchange anisotropy has been much less studied.[10] Reference 7 has mentioned in page 77 that there is no experimental evidence for the existence of this kind of anisotropy. Recently, UNiGe has shown strong indication for the presence of this anisotropic interaction.[11] We can expect that new compounds will be discovered as part of the fast advance that experimental magnetism is currently facing in the synthesis of new materials.

The simplest Hamiltonian describing anisotropic exchange interactions (exchange anisotropy) is the one-dimensional (1D) *XXZ* Heisenberg model

$$H_{XXZ}^{1D}=-J\sum_i\left(S_i^xS_{i+1}^x+S_i^yS_{i+1}^y+\Delta S_i^zS_{i+1}^z\right), \tag{1}$$

where $J>0$ and $\Delta>1$ (i.e., easy-axis anisotropy). For simplicity we will write Eq. (1) as

$$H_{XXZ}^{1D}=H_{isot}^{1D}-J\delta\sum_i S_i^zS_{i+1}^z, \tag{2}$$

where H_{isot}^{1D} is the one-dimensional isotropic Heisenberg Hamiltonian and $\delta\equiv\Delta-1>0$. Recently, Yamanaka and Koma[10] have used this model to describe the formation of a DW in a system in *any* dimension. However, as will be demonstrated, the treatment of the anisotropic exchange interactions deserves a more careful attention and, the effective one-dimensional Hamiltonian of the problem for $D>1$ is *not* the Hamiltonian (1). In fact, the effective Hamiltonian must contain an additional on-site anisotropy contribution whose role has been ignored for $D>1$. This contribution has its origin in the nonlocal character of the exchange anisotropy. On physical grounds, it contains the information about each neighbor spin out of the chains that support the domain structure. It is our main purpose to show the correct derivation of the 1D-effective Hamiltonian from the D-dimensional *XXZ* model and obtain a closed expression to the effective width of the wall using both the variational[8] and semiclassical[9] approaches. Our results will be compared to those obtained in Ref. 10 and to earlier reported numerical Monte Carlo data.[14] In closing, we will consider previous theories concerning the DW contribution to magnetoresistance in connection to the present work.

Our starting point will be the D-dimensional *XXZ* Heisenberg model

$$H^D_{XXZ} = H^D_{isot} - J\delta \sum_{\langle \mathbf{a},\mathbf{b}\rangle} S^z_{\mathbf{a}} S^z_{\mathbf{b}}, \tag{3}$$

where the sum goes over all bounds between nearest neighbors. We will be interested in solutions with the boundary conditions $\lim_{a_x \to \mp\infty} \mathbf{S_a} = S(0,0,\pm 1)$, a π DW in the x direction. Therefore, the magnetization on the sample will look the same along any spin chain in the y direction [two-dimensional (2D) case] or both y and z directions [three-dimensional (3D) case].

The effective one-dimensional Hamiltonian can be obtained using the fact that $S^\alpha_{\mathbf{b}} = S^\alpha_{\mathbf{a}} (\alpha = x,y,z)$ for every nearest neighbor of the spin in the **a**th site, except for the ones on the x axis. After summing over the sites out of the chains in the x direction, the Hamiltonian (3) reduces to the 1D version

$$\begin{aligned} H^{1D}_{eff} &= H^{1D}_{isot} - J\delta \sum_i S^z_i S^z_{i+1} - J\delta(D-1)\sum_i S^{z2}_i \\ &= H^{1D}_{XXZ} - J\delta(D-1)\sum_i S^{z2}_i. \end{aligned} \tag{4}$$

As can be seen, the one-dimensional effective Hamiltonian (4) coincides with the 1D version of the *XXZ* model *only* in the obvious case $D=1$. For $D>1$, the exchange anisotropy leads to an additional effective on-site contribution depending on D. We notice that H^D_{isot} also leads to a similar *but* isotropic contribution depending on S^2_i which cannot affect the form of the wall. In the usual case studied in Refs. 8 and 9, the effective one-dimensional Hamiltonian is simply the 1D version of the original D-dimensional model because the anisotropy is assumed to be of the on-site type. The additional on-site term in (4) makes the form and the width of the wall dependent on the system dimension or on the coordination number of the crystal structure.

The modification of the DW profile induced by the new terms can be obtained following a variational approach as in Ref. 8. A crystalline on-site anisotropy given by $-J\delta_c \Sigma_i S^{z2}_i$ can be added to (4) in order to consider a more general situation. We assume small values of δ and δ_c so that the continuum limit makes sense. Then, Eq. (4) with the crystalline on-site term added, defines the one-dimensional variational problem given by

$$\int \left(\frac{J}{2}(\partial_x \mathbf{S})^2 + \frac{J\delta}{2}(\partial_x S^z)^2 - J\delta_t S^{z2}_i \right) dx = \min, \tag{5}$$

where $\delta_t \equiv \delta D + \delta_c$ is the total anisotropy parameter depending on D and x is in units of the lattice constant.

As it is shown in (5), the exchange is anisotropic and the on-site interaction depends on the system dimension. Therefore, the DW profile and its effective width are different from those obtained in Ref. 8. As mentioned before, the on-site term reflects the fact that each site effectively feels the cost of energy to have its nearest neighbors pointing in directions away from the anisotropy axis. As the number of nearest neighbors increases with the dimension we can expect the effective width of the wall to decrease for higher D.

Using the angle representation for the magnetic moments

$$\mathbf{S}(x) = S\,[0, \sin\,\theta(x), \cos\,\theta(x)], \tag{6}$$

where we assume $S \gg 1$, Eq. (5) becomes

$$\int \left[\frac{1}{2}(1 + \delta \sin^2\,\theta)\theta'^2 - \delta_t \cos^2\,\theta \right] dx = \min, \tag{7}$$

which generates the equation of motion

$$\left(\frac{\delta\theta'^2 - 2\delta_t}{2} \right) \sin 2\theta + (1 + \delta \sin^2\,\theta)\theta'' = 0. \tag{8}$$

Integration of (8) with the boundary conditions of a π-DW leads to the solution for the magnetic structure of the form

$$\begin{aligned} -\sqrt{2(\delta D + \delta_c)}\, x = &\operatorname{arctanh}\left[\frac{\cos\,\theta(x)}{\sqrt{1 + \delta \sin^2\,\theta(x)}} \right] \\ &+ \sqrt{\delta} \arctan\left[\frac{\sqrt{\delta}\cos\,\theta(x)}{\sqrt{1 + \delta \sin^2\,\theta(x)}} \right]. \end{aligned} \tag{9}$$

As can be seen, the standard Landau and Lifshitz[8] expression $\cos\,\theta(x) = -\tanh(\sqrt{2\delta_c}\, x)$ can be obtained from Eq. (9) for $\delta = 0$. Equation (9) is thus the generalization of that expression for the case of anisotropic exchange interactions.

The same expression for the DW profile can be obtained following a different approach, as in Ref. 9. In that case, the static solution of the spin-quantum equations of motion,

$$\frac{dS^\alpha_{\mathbf{a}}}{dt} = 0 = \frac{1}{i\hbar}[S^\alpha_{\mathbf{a}}, H], \tag{10}$$

is considered. Here H can be either the D-dimensional Hamiltonian (3) or the effective one-dimensional Hamiltonian (4). The sum over the nearest neighbors of the **a**th spin resulting from (10) can be transformed in the continuum limit as

$$\sum_{\mathbf{b}} S^\alpha_{\mathbf{b}} \to \partial^2_x S^\alpha(x) + 2\,D\,S^\alpha(x). \tag{11}$$

For the case of the effective one-dimensional Hamiltonian (4), D must be taken equal to 1 in Eq. (11). Then the classical vector representation (6) can be used and Eq. (8)—and thus Eq. (9)—is recovered. We note that according to Eq. (6) one finally takes $S^x(x) = 0$. Thus, only the evolution of $S^x_{\mathbf{a}}$ actually needs to be considered in Eq. (10).

We can extract the effective width of the wall (W) from the behavior of Eq. (9) near the origin. For $x \to 0$ we get $\sqrt{1+\delta}\cos\,\theta(x) = -\sqrt{2(\delta D + \delta_c)}\, x$ and, therefore,

$$W = 2\sqrt{\frac{1+\delta}{2\delta_t}} = 2\sqrt{\frac{1+\delta}{2(\delta D + \delta_c)}}. \tag{12}$$

As expected, an increase in the dimension results in a narrower DW. This is in agreement with the fact that the local field produced by the spins out of a given chain increases the energy cost of the spin twist. As a consequence, the system effectively gets less spins out of the z axis and thus the effective width of the wall becomes smaller. The specific behavior $\propto 1/\sqrt{\delta_t}$ agrees with the limiting case $\delta \to 0$, in which the anisotropic exchange term $(J\delta/2)(\partial_x S^z)^2$ in Eq. (5) can be neglected. In that case, one gets an isotropic exchange

parameter $J/2$ and an on-site anisotropy with the effective parameter $J\delta_t$. The ratio of these two parameters determines[8] the effective width of the wall. Slightly away from that limit, Eq. (12) shows an additional exchange-type dependence on δ (i.e., δ is in the numerator) coming from the total exchange parameter $1+\delta=\Delta$ of the z components in the XXZ model.

When $\delta=0$, Eq. (12) gives $2(1/\sqrt{2\delta_c})$, which has no dependence on D and is the effective width of the wall in the well-known case for which the anisotropy in the original model is of the on-site type.[8,9] As can be seen from (12), the effective width has less sensitivity to variations in the parameter δ than in δ_c. This is a consequence of the combined role of δ as exchange and anisotropy parameter at the same time, as can be seen from the original model (3).

Now we are going to compare our results for $D=1$ with those obtained in Ref. 10, where $\delta_c=0$ was considered. Following a pure quantum method in treating the XXZ model (1), Yamanaka and Koma[10] rederived the Landau and Lifshitz expression $\cos\theta(x)=-\tanh(x/\lambda)$ with an effective wall width given by

$$2\lambda = -2\frac{1}{\ln q}, \tag{13}$$

where $0<q<1$ and $q+1/q=2\Delta$.

As discussed above, we can get such an expression for the domain wall profile, which corresponds to the case of isotropic exchange interactions and on-site anisotropy, *only* in the limited case $\delta\to 0$. Indeed, it is not hard to see that for $D=1$ and $\delta\to 0$, Eq. (9) —with $\delta_c=0$—reduces to that expression with λ given by $1/\sqrt{2\delta}$.

At first sight the DW width (13) looks quite different from our result given by Eq. (12), with $\delta_c=0$, in the $D=1$ case. However, as can be seen they also coincide for small values of δ ($\Delta\approx 1$). One first notices that since $\Delta>1$, then $q=\Delta-\sqrt{\Delta^2-1}$. We can expand Eqs. (12) and (13) in powers of δ and obtain for both cases $2/\sqrt{2\delta}+\mathcal{O}(\delta^{1/2})$.[12] Thus up to leading order in $1/\delta$, both the expression (12), with $\delta_c=0$, and the one reported in Ref. 10 are equal to $2(1/\sqrt{2\delta})$. It is interesting to note that Eq. (9) for the form of the wall and (12) for the effective DW width have been derived for large values of spin S. However, both of them reduce, for $D=1$ and small values of the parameter δ, to the results of Ref. 10 for spin $S=1/2$.

The anisotropic Heisenberg model has been studied before using the Monte Carlo method.[13] Recently, Serena and Costa-Krämer[14] have made use of this technique to describe a π DW in the XXZ model. In order to compare our results with theirs, we first make the equivalence between our parameters and those used in Ref. 14. Hereafter, to avoid confusion with Δ in the present work, we identify the anisotropy parameter of Ref. 14 by Δ'. One can see that they are related by $\Delta=1/(1-\Delta')$. Therefore, $\delta=\Delta-1=\Delta'/(1-\Delta')$and, from (12), with $\delta_c=0$, we get

$$W = \pi\frac{1}{\sqrt{2\,\Delta'\,D}}. \tag{14}$$

Here, the factor 2 of Eq. (12) has been changed to π to follow the definition used in Ref. 14 for the effective DW width. Equation (14) gives W in a simpler manner than the one given by Eq. (12) for $\delta_c=0$. Additionally, it looks closer to the result $\pi(1/\sqrt{2\delta_c})$ of the usual case of isotropic exchange interactions and on-site anisotropy. Equation (14) confirms the power-law $W\propto\Delta'^{-1/2}$ that has been suggested in Ref. 14. It also elucidates the fact that the proportionality factor of this behavior is determined by the dimensionality D of the system.

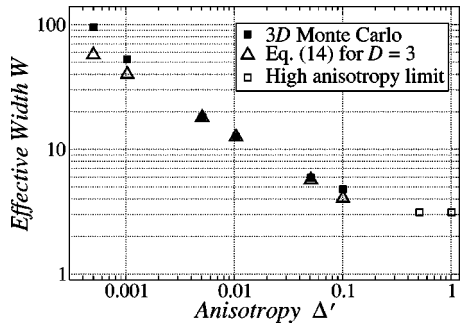

FIG. 1. The effective DW width, as obtained from Eq. (14) for $D=3$ (open triangles), is compared to Monte Carlo data (filled squares) from Ref. 14. Open squares correspond to the high anisotropy limit for which Eq. (14) is not applicable. Please see text for further details.

Figure 1 compares the effective DW width, as obtained from Eq. (14), to the numerical data from Ref. 14 for the case $D=3$. Here some remarks are in order. Equation (14) has been derived in the continuum limit, i.e., large values of W and thus small anisotropy values have been assumed. We need $\Delta'\ll 1/(2\,D)$ in Eq. (14) to get $W\gg 1$. Therefore, for $D=3$, we can expect Eq. (14) to give good results for $\Delta'\ll 1/6\approx 0.2$. This agrees with the fact observed by Serena and Costa-Krämer that for anisotropy values larger than $\Delta'=0.5$, the magnetization suddenly changes in one lattice constant.[14] The value $W=\pi$ has been defined in Ref. 14 for this high anisotropy limit. Open squares in Fig. 1 correspond to this case and are not considered in Eq. (14). An unexpected departure from Eq. (14) is observed for Monte Carlo (MC) data with very small anisotropy values. According to Ref. 14, this may be associated with numerical uncertainties for such very low values of anisotropy ($\Delta'<0.001$). With these comments in mind, we conclude that our results are in very good agreement with the numerical data of Serena and Costa-Krämer.

Previous theories have considered the role of a DW in the transport properties of ferromagnetic metals. The effective width W, when compared to the Fermi wavelength λ_F, determines how strong the effect of the DW is in increasing[2,4] or decreasing[3] the electrical resistance. Recently, Sil and Entel[15] have considered the modification of the electronic band structure by the DW and shown that there can be an increase or decrease of the resistance depending on the dimensionality, position of the Fermi energy, and strength of the coupling between conduction electrons and DW. The role of D has been considered through the modification of the density of states. One can see that these theories have considered no dependence of the effective DW width on the dimensionality D of the system. Here we have seen that this is valid only for

the usual case of isotropic exchange interactions and on-site anisotropy. This Brief Report reveals that the wall profile itself contains an additional D dependence for the case of anisotropic exchange interactions. In this case Eq. (12) will define such a D dependence of W, which is the relevant DW parameter in the electronic transport.

To summarize, we have followed both the variational and semiclassical approaches to describe a π DW in the XXZ model in a D-dimensional system. It was shown that the effective one-dimensional Hamiltonian contains an on-site anisotropy contribution which has been previously ignored for $D>1$. The standard Landau-Lifshitz DW profile for isotropic exchange interactions has been generalized. Increasing the dimension of the system decreases the width of the wall. This case is thus essentially different from the well known one for which the anisotropy in the original model is only of the on-site type. Very good agreement with earlier numerical data was found. This work adds a new source of D dependence for measurable physical properties like the magnetoresistance.

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