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Spin wave interaction with topological defects

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Abstract
Following our earlier gauge field theory analysis of the diffusion and interactions of classical and quantum waves with topological defects in solids (screw and edge dislocations), we present the analysis of the interaction of a classical spin wave with a screw dislocation studied within the Heisenberg ferromagnet model in which spins are located on a lattice containing dislocations. We show that the spin wave interaction with the screw dislocation shows a similarity to the Aharonov–Bohm-like deflection found previously for scattering of acoustic waves on the same type of defects.

One of the early applications of gauge field theory in condensed matter physics was that which described the influence of the frozen-in elastic distortions of the crystalline lattice due to topological defects, for example dislocations, on various other elastic properties of the crystal [1]. This formulation turned out to be equivalent to the differential geometry approach developed by Kröner [2]. In the recent publication [3] we compared [1] with other uses of gauge field theory in the theory of dislocations [4–6]. In the theory [1] one assumes Euclidean symmetry of the elastic energy density in the undistorted defect-free 'reference' state. The gauge group consists then of linear transformations of the Lagrange coordinates, representing the positions of material points in the reference state, at constant Euler coordinates which represent the displaced positions in the strained material. Due to this [1, 3] incorporate some important nonlinear couplings between dislocation-induced and otherwise generated distortions missing from [4–6]. Those couplings turn out to be essential in the analysis of diffusion [7] or sound propagation in a crystal with dislocations [3, 8]. The continuum gauge field theory of dislocations [1] has been used to analyse also the quantum particle dynamics in the crystal containing both edge and screw dislocations [10–12]. The scattering of quantum particles on the screw dislocations have also been discussed in [9] following the differential geometry formulation of the defects theory [2].

In [11] we have shown a systematic procedure to derive the Schrödinger equation from a microscopic lattice model, in that case a tight binding one, which is identical to that following from the use of the gauge field theory approach [13, 1, 3]. That procedure relies on a generalization of the expansion procedure leading from the lattice (discrete) to the continuum description of the medium properties, which consists of formal $\mathcal{O}(a^2)$ expansion in the bare lattice constant and $\mathcal{O}(\boldsymbol{\beta}^2(\boldsymbol{x}))$ expansion in the Kröner distortions $\boldsymbol{\beta}$ describing topological defect distributions in the lattice.

In this paper we report the results of the procedure [11] applied to the classical, nearest-neighbour, isotropic Heisenberg magnet model residing on a lattice containing dislocations. We shall formulate here the general theory and show exact results for the spin wave interaction with a frozen-in distortion due to a screw dislocation. That allows us to elucidate the difference between our theory and the earlier work of Kutchko and collaborators [15, 16]. The analysis of the modifications due to the phonon coupling will be discussed elsewhere.

The Landau–Lifshitz equation for a spin vector field $\boldsymbol{S}(\boldsymbol{x})$:

$$\partial_t \boldsymbol{S}(\boldsymbol{x}) = Ja^2 \boldsymbol{S}(\boldsymbol{x}) \times \nabla^2 \boldsymbol{S}(\boldsymbol{x}) \qquad (1)$$

after linearization around static and constant 'magnetization' S_0 describes spin waves with dispersion relation $\omega(\boldsymbol{q}) = Ja^2 S_0 \boldsymbol{q}^2$. Equation (1) follows from the continuum approximation ($\mathcal{O}(a^2)$; $a \to 0$ expansion) of the equations of motion for classical spins described by the classical Heisenberg ferromagnet Hamiltonian:

$$\mathcal{H} = \frac{1}{2} \sum_{n,a(n)} J(\boldsymbol{n}, \boldsymbol{n} + \boldsymbol{a}(\boldsymbol{n}))\boldsymbol{S}(\boldsymbol{n}) \cdot \boldsymbol{S}(\boldsymbol{n} + \boldsymbol{a}(\boldsymbol{n})) \qquad (2)$$

where the vector $\boldsymbol{n}$ denotes a simple cubic lattice site position, $\{\boldsymbol{a}_\alpha(\boldsymbol{n})\}$; $\alpha = 1, \ldots, d$ is the set of the lattice vectors and $\boldsymbol{S}(\boldsymbol{n})$ the spin vector on that site. $J(\boldsymbol{n}, \boldsymbol{n} + \boldsymbol{a}(\boldsymbol{n}))$ denotes the nearest-neighbour exchange interaction. In the undistorted lattice, in some coordinate system, $a^i_\alpha(\boldsymbol{n}) = a\delta^i_\alpha$, where a is the bare lattice constant.

Consider now a distorted lattice. Defects caused Kröner lattice distortions $\beta^i_j(\boldsymbol{n}) = B^i_\alpha(\boldsymbol{n})\delta^\alpha_j - \delta^i_j$, known for essentially all topological defects [2], change the global equivalence of the set of the lattice vectors $\{\boldsymbol{a}_\alpha(\boldsymbol{n})\}$. To carry out the sum in equation (2) we use the procedure discussed in [11] of decomposing that set into $\{\boldsymbol{a}^+_\alpha(\boldsymbol{n}), \boldsymbol{a}^-_\alpha(\boldsymbol{n})\}$, where $\boldsymbol{a}^-_\alpha(\boldsymbol{n})$ are essentially opposite to $\boldsymbol{a}^+_\alpha(\boldsymbol{n})$ (in the sense of the distorted lattice geometry). To the second order in $\boldsymbol{B}_\alpha$ we have [11]

$$\boldsymbol{a}^\pm_\alpha(\boldsymbol{n}) = \pm a\boldsymbol{B}_\alpha(\boldsymbol{n}) + \frac{a^2}{2}\left(\boldsymbol{B}_\alpha(\boldsymbol{n}) \cdot \frac{\partial}{\partial \boldsymbol{n}}\right)\boldsymbol{B}_\alpha(\boldsymbol{n}), \tag{3}$$

and subsequently up to $\mathcal{O}(a^2, \boldsymbol{B}_\alpha)$

$$\boldsymbol{S}(\boldsymbol{n} + \boldsymbol{a}^\pm_\alpha(\boldsymbol{n})) = \boldsymbol{S}(\boldsymbol{n}) \pm a\left(\boldsymbol{B}_\alpha(\boldsymbol{n}) \cdot \frac{\partial}{\partial \boldsymbol{n}}\right)\boldsymbol{S}(\boldsymbol{n}) + \frac{a^2}{2}\left(\boldsymbol{B}_\alpha(\boldsymbol{n}) \cdot \frac{\partial}{\partial \boldsymbol{n}}\right)^2 \boldsymbol{S}(\boldsymbol{n}). \tag{4}$$

In the limit $a \to 0$ the matrix fields $\boldsymbol{B}_\alpha$ and its inverse $B^i_\alpha B^\alpha_j = \delta^i_j$ provide the continuum description of the distorted crystal by a Riemann–Cartan manifold with the metric tensor $g_{ij} = \delta_{\alpha\beta}B^\alpha_i B^\beta_j$ and affine connection $\Gamma^k_{ij} = B^k_\alpha \partial_i B^\alpha_j$ [2, 11]. Using that interpretation we can rewrite the $\mathcal{O}(a^2, \boldsymbol{\beta}^2)$ Heisenberg Hamiltonian (2) in the covariant form

$$\mathcal{H} = \frac{Ja^2}{2}\int \mathrm{d}^d x\sqrt{g}g^{ij}\boldsymbol{S}(\boldsymbol{x}) \cdot \nabla_i\nabla_j\boldsymbol{S}(\boldsymbol{x}), \tag{5}$$

where $g = \det g_{ij}$, g^{ij} is the inverse of g_{ij} and ∇_i denotes covariant derivative with respect to connection Γ^k_{ij}. In (5) we have retained only those terms in the Hamiltonian (2) expansion which correspond to the exchange interaction J independent of the lattice position. Note that the Hamiltonian (5) describes the purely topological in nature interaction between the dislocation and magnetization $\propto \boldsymbol{S}(\boldsymbol{x})$ via the differential geometric structure of the effective Riemann–Cartan manifold describing the medium with defects.

In a real crystal one should also include two additional couplings between the magnetic degrees of freedom and the crystalline lattice. Both of them will contribute non-covariant terms to the Hamiltonian (5). The first one is due to the localized change in the exchange integral $J(\boldsymbol{n})$ caused by the presence of the dislocation core. The second one is caused by the magnetostriction, that is the dependence of J on the lattice vibration phonons described by the field $\boldsymbol{u}(\boldsymbol{n})$:

$$J(\boldsymbol{n}, \boldsymbol{n} + \boldsymbol{a}(\boldsymbol{n})) \to J(\boldsymbol{n}, \boldsymbol{n} + \boldsymbol{a}(\boldsymbol{n})) + \gamma \cdot (\boldsymbol{u}(\boldsymbol{n}) - \boldsymbol{u}(\boldsymbol{n} + \boldsymbol{a}(\boldsymbol{n}))), \tag{6}$$

where $\gamma = \partial J(\boldsymbol{n})/\partial \boldsymbol{n}$.

Inserting this expansion into the Hamiltonian (2) we found that the lowest-order, nonvanishing, in $a^2, \boldsymbol{\beta}^2$ term in the $\boldsymbol{u} - \boldsymbol{S}$ coupling contributes a term $\propto \boldsymbol{S}^2\gamma \cdot g^{ij}\nabla_i\nabla_j\boldsymbol{u}$ to the Hamiltonian density. Since $\boldsymbol{S}^2$ is the constant of motion for the Heisenberg model there are no corrections to the equations of motion for spin components resulting from that term. This is reminiscent of the complete integrability of the compressible Heisenberg model (2) in $d = 1$ discussed in [14]. The nontrivial magnetostriction coupling between the phonon's and the spin degree of freedom appears in higher order with respect to a^2.

The coupling discussed above between the topological defects and the spin degrees of freedom distinguishes our model from that used in [15, 16] in which the coupling between the dislocation caused lattice distortion and the spins were described by the term in the Hamiltonian density of the form $\propto \sigma^D_{ij}S^iS^j$, where σ^D_{ij} stands for the stress tensor in the elastic medium due to the localized dislocation [17]. The latter term was added to the usual Heisenberg Hamiltonian by phenomenological arguments which are not born out by our, microscopic in origin, analysis.

To describe the coupling between spins, dislocation-induced distortion and phonons, we have to employ the gauge field formulation for both spin and phonon fields. The latter dynamics was discussed in [3]. Using those results we have to add to the Hamiltonian density in (5) the effective energy for the phonon field interacting with topological defects, namely

$$\delta\mathcal{H}(x, t) \equiv \tfrac{1}{2}[D_i u_\alpha(x, t)]C^{i\alpha j\beta}(x)[D_j u_\beta(x, t)], \tag{7}$$

where the gauge covariant derivative $D_i \equiv B^\alpha_i(x)\partial_\alpha$. The space-dependent coefficients $C^{i\alpha j\beta}(x) \equiv (B^\alpha_k(x)c^{ikjl}B^\beta_l(x) + S^{ij}(x)\delta^{\alpha\beta})$ are the effective elastic constants, replacing bare coefficients c^{ijkl}, and S^{kl} is the stress tensor due to the frozen-in defects $S^{kl} = \frac{1}{2}c^{klij}[B^\alpha_i(x)\delta_{\alpha\beta}B^\beta_j(x) - \delta_{ij}]$. We have shown in [3] that the solutions for the Lamé equations following from the phonon Hamiltonian (7) exhibit Aharonov–Bohm-like behaviour in the presence of the screw dislocation.

We shall show now that the same situation occurs for pure spin waves as described by the Hamiltonian (5). Using the spin Poisson brackets $\{S^a(\boldsymbol{x}), S^b(\boldsymbol{y})\} = (\delta(\boldsymbol{x} - \boldsymbol{y})/\sqrt{g})\epsilon^{abc}S^c(\boldsymbol{x})$ we found, from (5), that the covariant form of the Landau–Lifshitz equation of motion (1) is

$$\partial_t\boldsymbol{S}(\boldsymbol{x}) = Ja^2\boldsymbol{S}(\boldsymbol{x}) \times \hat{\mathcal{B}}\boldsymbol{S}(\boldsymbol{x}), \tag{8}$$

where $\hat{\mathcal{B}}$ denotes the wave operator:

$$\hat{\mathcal{B}} = g^{ij}[\nabla^{\mathrm{T}}_i\nabla_j + \nabla^{\mathrm{T}}_i T^k_{jk}]. \tag{9}$$

Here $\nabla^{\mathrm{T}}_i = \nabla_i + 2T^k_{ik}$ and $T^k_{ij} = \Gamma^k_{ij} - \Gamma^k_{ji}$ is the torsion tensor [1, 2].

Linearizing now equation (8) around a constant is the space stationary solution $\boldsymbol{S} = S_0\boldsymbol{e}_z$, we obtain the covariant equation for spin waves in the ferromagnet containing defects whose density is described by the Riemann–Cartan manifold torsion tensor T^k_{ij}. Writing $\boldsymbol{S}(\boldsymbol{x}, t) = \boldsymbol{S}_0 + \delta\boldsymbol{S}(\boldsymbol{x}, t)$ and introducing for convenience the complex amplitude $S_0\Psi(\boldsymbol{x}, t) = (\delta S_x(\boldsymbol{x}, t) + \imath\delta S_y(\boldsymbol{x}, t))$ we obtain the Schrödinger-like equation for Ψ, namely

$$\imath\partial_t\Psi(\boldsymbol{x}, t) = -\frac{1}{2\mu}\hat{\mathcal{B}}\Psi(\boldsymbol{x}, t) \tag{10}$$

where $\mu = 1/2Ja^2S_0$. Equation (10) is the spin wave analogue of the Kawamura equation [19, 20] which leads to the Aharonov–Bohm [18]-like solutions for the waves interacting with a defect.

Note that, as discussed above, relaxing our assumption made in equation (5) $J = \text{const}$, we would obtain additional terms in the Hamiltonian (5) which, following [11], we should call non-covariant. It follows from the Kawamura analysis and our previous work that it is the covariant term (5) which describes the fundamental properties of the topological interaction between the spin degrees of freedom and the lattice distortion. The non-covariant terms can then be treated by means of the perturbation theory as discussed in [12]. We shall return to these additional effects in a subsequent publication.

We shall now present the solution of equation (10) for a single screw dislocation along the z axis with the Burgers vector $\boldsymbol{b} = b\boldsymbol{e}_z$. The only nonvanishing components of the Kröner distortions β^i_j are then β^3_i, $i = 1, 2$:

$$\begin{aligned}\beta^3_1 &= -\frac{b}{2\pi}\partial_2 \ln\sqrt{(x^1)^2 + (x^2)^2} \\ \beta^3_2 &= \frac{b}{2\pi}\partial_1 \ln\sqrt{(x^1)^2 + (x^2)^2}.\end{aligned} \tag{11}$$

Assuming in the cylindrical coordinates $\Psi(r, \phi, z, t) = \chi(r, \phi)\exp(\text{i}kz + \text{i}\omega t)$ we found that the envelope $\chi(r, \phi)$ obeys the Aharonov–Bohm equation [18]:

$$\left[\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\left(\frac{\partial}{\partial\phi} + \imath\alpha\right)^2 - q^2\right]\chi(r, \phi) = 0, \tag{12}$$

where $\alpha = kb/2\pi$ and $q^2 = k^2 + 2\mu\omega$. Using the asymptotic $r \to \infty$ solution for that equation [12, 18–20] and recalling the definition of the function Ψ we found

$$\begin{aligned}\begin{pmatrix}\delta S_x \\ \delta S_y\end{pmatrix} &= S_0\begin{pmatrix}\cos \\ -\sin\end{pmatrix}(\alpha\phi + qr\cos\phi) \\ &+ \frac{\sin(\pi\alpha)}{\cos(\phi/2)\sqrt{2\pi qr}} \\ &\times \begin{pmatrix}\cos \\ \sin\end{pmatrix}(qr + \alpha(\phi - \pi)/2|\alpha| - \pi/4).\end{aligned} \tag{13}$$

In the absence of the dislocation the (pseudo)flux $\alpha = 0$ and we recover the standard spin wave solution of equation (1). The first term on the rhs of equation (13) shows the helical structure of the incoming spin wave due to global distortion of the lattice and the second describes the scattering phase shift due to the presence of dislocation. In figure 1 we have shown a Mathematica 7 generated density plot for the δS_y component of the solution (13). The δS_x component exhibits an identical structure with a trivial phase shift found from (13).

The above-presented solution for the spin waves propagating on a lattice containing a screw dislocation completes our analysis of how the topological defects, such as dislocations, modify the wave phenomena in solids [3, 10–12]. The analysis has been systematically carried out within the scope of the gauge field theory formulation of the defect theory from [1]. The most significant result of that endeavour is that the Aharonov–Bohm-like oscillation are prevailing in all wave phenomena in condensed matter where the medium carrying waves can be modelled as the manifold with a torsion sharing topological similarity with the simple case discussed in the pioneering work [18]. Since the description we use is directly borrowed from field theory and general relativity [5, 13] it is tempting to suggest that this should also be the case in the other applications, for example propagation of the gravitational waves in the universe with torsion. The anisotropy discussed in [12] of the scattering cross section for matter waves on the screw dislocation, resulting from the non-covariant part of the Hamiltonian caused by the local deformation of the medium next to the defect core, might also be a new and important property for general relativity applications.

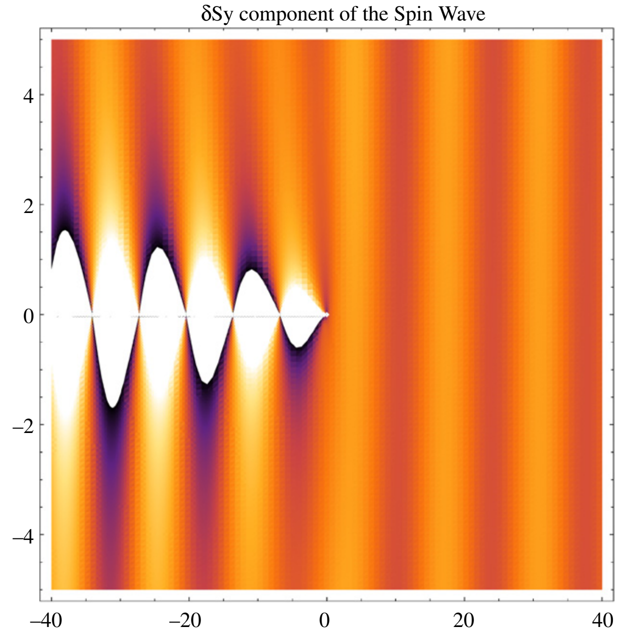

Figure 1. Mathematica 7 density plot for spin wave S_y solution equation (13). The wave is approaching from the right and deflects from the screw dislocation line located at the origin and perpendicular to the plot surface. The wavy edges of the cut to the left from the dislocations show the Aharonov–Bohm-like oscillations determined by the (pseudo)flux $\alpha = 0.4$.

(This figure is in colour only in the electronic version)

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