Acta Universitatis Carolinae. Mathematica et Physica

Z. Chvoj

Remark to the linear model of a ferromagnetic with defects

Acta Universitatis Carolinae. Mathematica et Physica, Vol. 14 (1973), No. 2, 9--12

Persistent URL: http://dml.cz/dmlcz/142307

1973 ACTA UNIVERSITATIS CAROLINAE - MATHEMATICA ET PHYSICA VOL. 14, NO. 2 Pag. 9–12

Remark to the Linear Model of a Ferromagnetic With Defects

Z. CHVOJ
Department of Theoretical Physics, Charles University, Prague

Received 23 January 1973

Recently several papers have appeared dealing with the influence of the impurity and of the external conditions in the model of spin waves and their energetic spectrum in thin films, as e.g. in [2]. These authors have limited themselves to the case of one

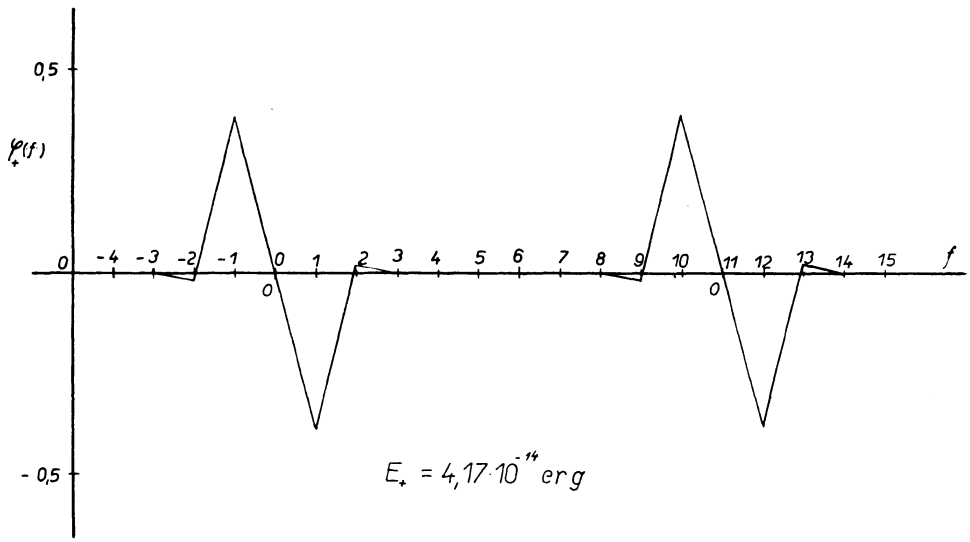

Fig. 1. The spin wave function according to [2].

impurity atom in the linear model of a ferromagnetic in their work. When calculating the energy spectrum of the spin waves, they start from the spin Hamiltonian containing the Heisenberg exchange term, the Zeeman term and the axial anisotropy term

$$H = H_0 + V,$$

where

$$H_0 = -(1/2)\,\mathcal{J} \sum_{f,g} \vec{S}_f \vec{S}_g - \mu_0 g H_e \sum_f S_f^z,$$

and

$$V = \mathcal{J} \sum_{\delta} \vec{S}_0 \vec{S}_\delta - \gamma \mathcal{J} \sum_{\delta} \vec{S}_0 \vec{S}_\delta - \mu_0 g H_e (S'^z_0 - S^z_0) - K(\mathcal{J}/2) \sum_{\delta} (S^z_\delta)^2 ,$$

f, g, δ indicate the positions of the spins (adding over the nearest neighbours), K is coefficient of the axial anisotropy. The impurity has been located in the position o with the spin $S' = \sigma^2 S$ and the exchange integral with the nearest neighbours $\mathcal{J}' = \gamma \mathcal{J}$.

In the calculation Born–Kármán boundary conditions have been used. However, the results obtained in that way are independent from the position of the impurity in the chain and the effect caused by the change of the number of the nearest neighbours if the impurity atom is placed near to the surface of the ferromagnetic is lost. The results in [2] have been obtained by the perturbation method (the perturbation being the interaction energy V) in the first approximation, while a symmetrical solution of spin waves has not been taken into consideration. The

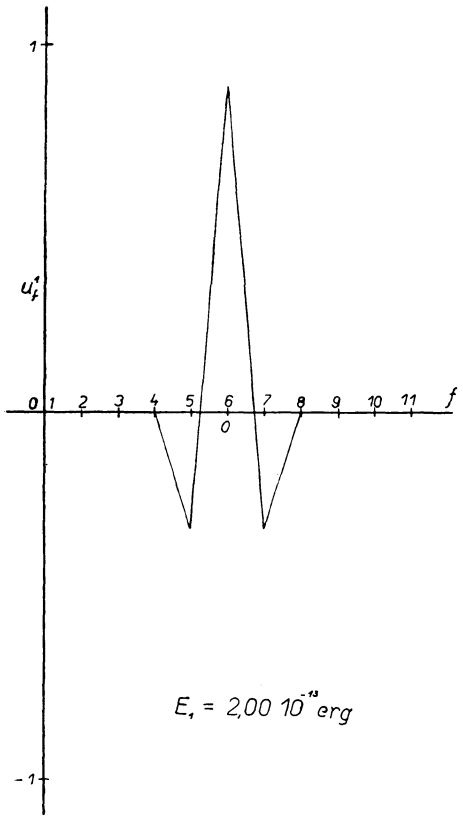

Fig. 2. The symmetrical spin wave function according to [1] if the impurity atom lies inside of the chain

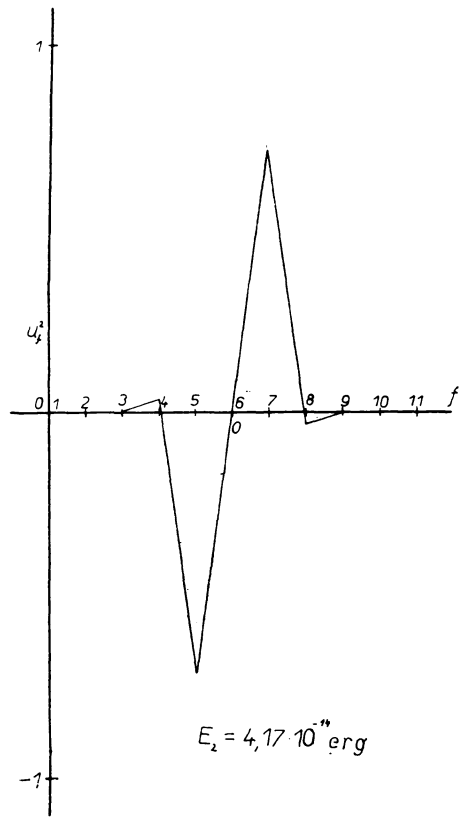

Fig. 3. The antisymmetrical spin wave function according to [1] if the impurity atom lies inside of the chain

energy corresponding to the impurity is situated above (E_+) or below (E_-) the lowest band. In this calculation the wave function ($\varphi_+(f)$ resp. $\varphi_-(f)$) of the relevant spin wave has also been determined. This function with the relevant eigen-value of the energy is given in Fig. 1.

Since the symmetrical solution of the spin waves has not been included in [2] and the change of the number of the nearest neighbours near the surface of the ferromagnetic has not been taken into account and since, moreover, the model used in [2] is a special case of the model used in [1] we have re-examined the results of [2] using the procedure of [1]. In which case the perturbation theory is not used, the diagonalisation being done exactly. It is, therefore, interesting to see what is the difference of the results of both calculation procedures. We use the Hamiltonian H containing the Heisenberg exchange term, the Zeeman term and the axial anisotropy term

$$H = -(1/2)\sum_{j,j'=1}^{N} \mathcal{J}_{j,j'}(\vec{S}_j, \vec{S}_{j'}) - \mu_0 g H_e \sum_{j=1}^{N} S_j^z + \sum_{j=1}^{N} k_j (S_j^z)\,.$$

We will find the energy spectrum of the system in the spi-wave approximation taking into account nearest neighbours only. The finite dimensions of the linear chain, i.e. the boundary conditions, have explicitely been taken into consideration and therefore the results depend now on the position of the impurity atom in the chain. So we obtain the energy eigen-values of the spin waves as eigen-values of the matrix

$$\begin{bmatrix}
\mathcal{J}_{1,2}S_2 - 2k_1S_1 - \mathcal{J}_{1,2}\sqrt{(S_1S_2)}\,, 0, \ldots\ldots\ldots\ldots\ldots\ldots\ldots, 0 \\
-\mathcal{J}_{2,1}\sqrt{(S_1S_2)}\,, \mathcal{J}_{2,1}S_1 + \mathcal{J}_{2,3}S_3 - 2k_2S_2, -\mathcal{J}_{2,3}\sqrt{(S_2S_3)}\,, 0, \ldots, 0 \\
\vdots \\
0, \ldots, 0, -\mathcal{J}_{i,i-1}\sqrt{(S_iS_{i-1})}\,, \mathcal{J}_{i,i-1}S_{i-1} + \mathcal{J}_{i,i+1}S_{i+1} - 2k_iS_i, - \\
\qquad\qquad -\mathcal{J}_{i,i+1}\sqrt{(S_iS_{i+1})}\;\; 0, \ldots, 0 \\
\vdots \\
0, \ldots\ldots\ldots\ldots\ldots, 0, -\mathcal{J}_{N,N-1}\sqrt{(S_NS_{N-1})}\,, \mathcal{J}_{N,N-1}S_{N-1} - 2k_NS_N
\end{bmatrix} \qquad (1)$$

The spin wave eigen-functions u_f^i are then the eigen-vectors of (1). The diagonalisation has been done numerically using a computer. These results as well as the programs needed for the numerical calculation are taken from the work [1].

The results of [2] have been compared with ours in which case the dependence on position of the impurity atom in the chain has been studied, (see Fig. 2, 3, 4). In the figures f – indicates the position of the atoms, O – atom of the impurity.

Hence, we see that both methods give the same results (within reasonable

limits of accuracy) for the antisymmetrical wave. The energy for the impurity atom placed inside of the chain becomes lower, if the impurity approaches to the surface. In case that the impurity atom becomes a surface atom, only the energy of the symmetrical spin wave may be observed above the lowest energy band. The energy

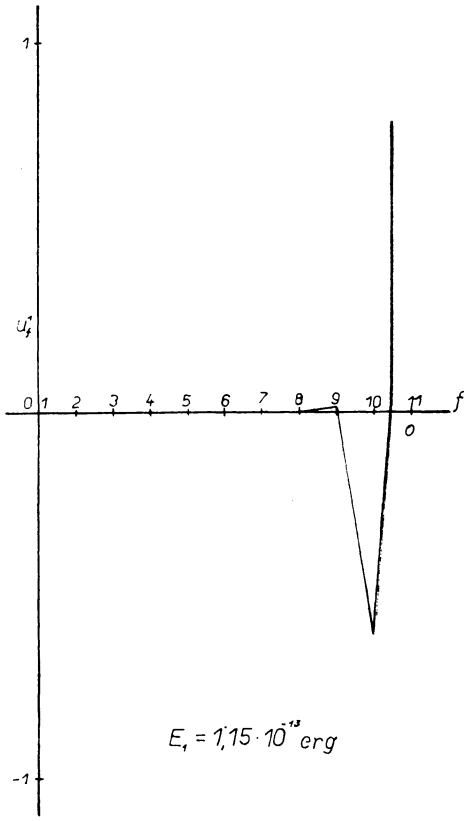

Fig. 4. The symmetrical spin wave function of the spin wave according to [1] if the impurity atom lies on the "surface" (i.e. one of the ends) of the chain

of the antisymmetrical wave is now in the band. These properties could not be obtained from [2], since here the periodic boundary conditions are used.

I thank to Professor L. Valenta for his kind guidance and the advices given to me when working on this paper and to Mrs. H. Šmydková for her help with the numerical calculation.

References

[1] Valenta L., Vamanu D., Havlasová H.: J. de Physique 32, Cl - 569 (1971).
[2] Sukiennicki A., Zagorski A.: Acta Physica Polonica, A 37, 429 (1970).