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Abstract. In this paper, we theoretically investigate the impurity state in a ferrimagnet. We consider a body–centered cubic crystal based on the model of two sublattices, A–sublattice and B–sublattice. The impurity spin (S_i) is assumed to be not located at the interstitial but located at the A–sublattice point or B–sublattice point. Confining our interests to the case of one impurity and one spin–wave, we solve our problem exactly. We have found several interesting features for our system. For example, the localized spin–wave appears in the band gap only when S_i is located at A–sublattice point if $S_A < S_B$ and the exchange coupling between the impurity spin and the neighboring S_B spin is antiferromagnetic.

1. Introduction

It is known that we can obtain the information concerning the physical states of the perturbation such as the surface by theoretically analyzing the experimental data on the localized spin waves [1,2]. In this paper, we develop a theory of spin waves in a ferrimagnet with impurities. Although both the experimental and theoretical investigations of ferro- and antiferromagnets including localized impurities have been widely performed [2,3], the theoretical study of ferrimagnets with impurities has not yet been made as far as we know. One of the main differences between ferrimagnetism and antiferromagnetism will be the existence of the gap between two bands. It will be worth to study how the localized spin waves at the impurity appear outside the bands, especially in the band gap.

2. Model and Calculation

Let us consider a body–centered–cubic ferrimagnet based on the model of two sublattices, up–sublattice and down–sublattice. The former and the latter are called A–sublattice and B–sublattice respectively. We confine our interests to the case of one impurity and one magnon. This will be experimentally relevant if the impurity concentration is very low and theoretically our problem can be solved exactly. We assume that the impurity spin is localized at one of the A–sublattice points. Our Hamiltonian is written as

$$H = 2J \sum_{j,n} \vec{S}_j \cdot \vec{S}_n (1 - p\, c_0^\dagger c_0)$$

where $\sum_{j,n}$ stands for the summation over the nearest neighbor site pairs. The lattice site 0 belongs to the A–sublattice. j denotes the A–sublattice sites and n denotes the B–sublattice sites throughout this paper. $c^\dagger$ and c are the creation and annihilation operators for the impurity at the lattice site 0. These operators follow the Fermi commutation relations. p is a numerical parameter. J is the exchange coupling between neighboring host spins and $J(1-p) = J'$ is the exchange coupling between the impurity and the neighboring B spin. The impurity spin is antiparallel to the neighboring spins if $p < 1$ and it is parallel to the neighboring spins if $p > 1$ in the ground state. When $p = 1$, our system is composed of isolated spin and a ferrimagnetic system with nonmagnetic hole. The magnitude of the spin operator S_j (S_n) is denoted by S_A (S_B). The magnitude of the impurity spin, S_i, is denoted by $S_i = S_A(1-q)$, where q is a numerical constant with $0 < q < 1$.

By using Holstein-Primakoff method, the spin operators are rewritten by the spin deviation operators; $S_j^z = S_A - a_j^\dagger a_j$, $S_j^- = \sqrt{2S_A} a_j^\dagger$, $S_j^+ = \sqrt{2S_A} a_j$, $S_n^z = -S_B + b_n^\dagger b_n$, $S_n^+ = \sqrt{2S_B} b_n^\dagger$, $S_n^- = \sqrt{2S_B} b_n$. Here a,
30 $a^\dagger$, b and $b^\dagger$ are Bose operators. For the impurity spin, $S_0^z = S_i - a_0^\dagger a_0$, $S_0^- = \sqrt{2S_i} a_0^\dagger$ and $S_0^+ = \sqrt{2S_i} a_0$ when $p < 1$ and $S_0^z = -S_i + a_0^\dagger a_0$, $S_0^+ = \sqrt{2S_i} a_0^\dagger$ and $S_0^- = \sqrt{2S_i} a_0$ when $p > 1$. Let us consider a one–magnon

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and one–impurity state which is defined by

$$\Psi = (\sum_j A_j a_j^\dagger + \sum_n B_n b_n) c_0^\dagger \mid 0 > .$$

Here $\mid 0 >$ denotes the spin wave ground state for the ferrimagnet in which neither magnons nor impurities exist.

Using Ψ and H in the Schrödinger equation, we obtain the secular equations for A_j and B_n. For the case $p < 1$, the secular equations are written as

$$(-U + 2JS_B z)A_j - 2JS_r \sum_\rho B_{j+\rho} + \delta(j,0)(-2JzS_B pA_j + 2JS_r(p + p'q') \sum_\rho B_{j+\rho}) = 0$$

$$(-U - 2JS_A z)B_n + 2JS_r \sum_\rho A_{n+\rho} + \delta(n, j + \rho_1)(2JS_A(p + p'q)B_n - 2JS_r(p + p'q')A_{n+\rho_1}) = 0$$

where U represents the energy measured from the ground state energy. z is the number of nearest neighbors and δ is the usual Kronecker's delta function. $S_r = \sqrt{S_A S_B}$ and ρ, ρ_1 denote the vectors directed between nearest neighbors. $p' = 1 - p$ and $q' = 1 - \sqrt{1-q}$. Introducing the Green functions, we can solve the above secular equations. The energy bands, $u^\pm = U^\pm/2JzS$, is obtained as

$$u^\pm = \frac{1}{2}\left[\sqrt{\beta} - \frac{1}{\sqrt{\beta}} \pm \sqrt{(\sqrt{\beta} - \frac{1}{\sqrt{\beta}})^2 + 4(1 - \gamma_k^2)}\right]$$

where $\beta = S_B/S_A$ and $\gamma_k = (1/z)\sum_\rho e^{ik\cdot\rho}$. In the following, we show the impurity–magnon bound states in the band gap for the case $\beta = 2$.

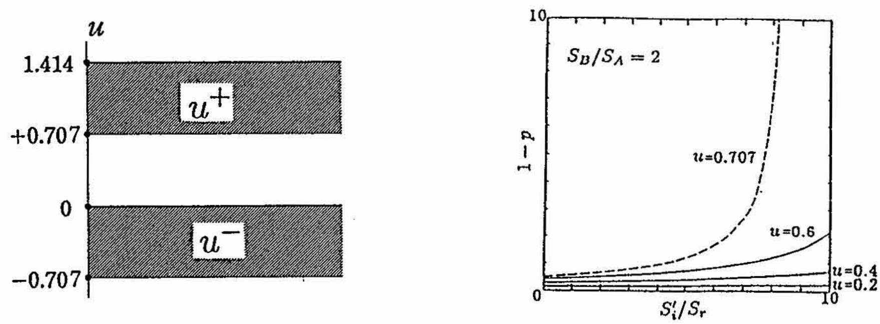

Fig.1 Impurity–magnon bound states in the band gap for the case of $\beta = 2$.

In this work, we have investigated localized spin wave states outside the continuous bands for various parameters. If the experiment for the localized spin waves at the impurity were performed, we may obtain useful information about the physical states of the impurity.

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