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REDUCED ZERO-POINT SPIN CONTRACTION IN IMPURE ANTIFERROMAGNETS

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Résumé. — Les propriétés d'un antiferromagnétique contenant des impuretés de substitution sont étudiées pour un spin d'impureté S' et pour une interaction I' portant sur des proches voisins. La contraction du point zéro du spin de l'impureté et de ses proches voisins est évaluée pour un couplage ferromagnétique ($I' > 0$) et antiferromagnétique ($I' < 0$). $\langle S^z \rangle$ est développé en perturbation en $1/z$, où z est le nombre de proches voisins. Des résultats numériques pour le cubique centré sont présentés. Dans le cas particulier d'une impureté non magnétique la contraction de point zéro du spin des proches voisins est moindre que celle d'un pur antiferromagnétique.

Abstract. — Impure antiferromagnets containing a substitutional foreign atom of spin S' coupled to its nearest neighbours by exchange coupling I' are considered. The zero-point spin contraction is calculated at the impurity site and at its first neighbours for ferromagnetically ($I' > 0$) as well as antiferromagnetically ($I' < 0$) coupled impurities. The calculation of $\langle S^z \rangle$ is performed in a perturbative way in powers of $1/z$, where z is the number of nearest neighbours. Numerical results are presented for bcc crystal. In the special case of nonmagnetic impurity the zero-point spin contraction on the first neighbours is reduced as compared to a pure antiferromagnet.

The problem of magnetic impurities in Heisenberg model ferro- and antiferromagnets has been extensively discussed recently, mostly from the point of view of the localized and virtual spin wave excitations. In antiferromagnets the disturbance around the impurity results in the modification of the zero-point spin contraction, too. This quantity has been investigated theoretically by Lovesey [1], van de Braak [2] and Tonegawa [3] for nonmagnetic and antiferromagnetically coupled impurities, respectively. Lovesey obtained an increased contraction on the first neighbours of a nonmagnetic impurity, while the two other authors a reduced one. In these papers the Holstein-Primakoff transformation or the decoupling of the Green function equation of motion has been applied. Our aim was to investigate this problem using the perturbation theory for the spin operators proposed by Vaks, Larkin and Pikin [4].

Substituting an atom by an impurity of spin S' on the spin down sublattice of a Heisenberg model antiferromagnet with exchange coupling I' between the impurity and its first neighbours, we have calculated $\langle S^z \rangle$ for the impurity site and for the first neighbours. Both ferromagnetic ($I' > 0$) and antiferromagnetic ($I' < 0$) coupling have been considered.

The expansion parameter in our calculation is $1/z$, where z is the number of nearest neighbours. It has to be taken into account in the expansion that the contribution from every momentum sum is proportional to $1/z$. Denoting by $\langle S_\delta^z \rangle$ the magnetic moment on the first neighbours of the impurity the first order correction is Anderson's spin wave result [5] and the first correction due to the presence of the impurity appears in second order. Quoting only the final results

$$\begin{aligned} \langle \Delta S_\delta^z \rangle &\equiv \langle S_\delta^z \rangle - \langle S^z \rangle_{\text{And}} = \\ &= \frac{1}{zN} \sum_k \frac{1 - \sqrt{1 - \gamma_k^2}}{1 + \sqrt{1 - \gamma_k^2}} + \frac{\alpha\beta}{zN} \sum_k \frac{1 - \sqrt{1 - \gamma_k^2}}{1 + \sqrt{1 - \gamma_k^2}} \cdot \frac{1}{\sqrt{1 - \gamma_k^2}} \\ &\quad - \frac{\alpha^2 \beta}{zN} \sum_k \left(\frac{1}{\sqrt{1 - \gamma_k^2}} - 1 \right) \frac{1 - \sqrt{1 - \gamma_k^2}}{\alpha - \sqrt{1 - \gamma_k^2}} - 2 \frac{1 - \alpha}{1 + \alpha} \quad (1) \\ &\quad \times \frac{\alpha^2 \beta}{zN} \sum_k \frac{\gamma_k^2}{1 - \alpha^2 - \gamma_k^2} - \frac{1}{z^2} \left(\frac{1}{4} - \frac{\alpha^2 \beta}{(1 + \alpha)^2} \right) \end{aligned}$$

for antiferromagnetic coupling, and

$$\begin{aligned} \langle \Delta S_\delta^z \rangle &\equiv \langle S_\delta^z \rangle - \langle S^z \rangle_{\text{And}} = \\ &= \frac{1}{zN} \sum_k \frac{1 - \sqrt{1 - \gamma_k^2}}{1 + \sqrt{1 - \gamma_k^2}} - \frac{1}{4z^2} + \\ &\quad + \frac{\alpha\beta}{zN} \sum_k \frac{1 - \sqrt{1 - \gamma_k^2}}{1 + \sqrt{1 - \gamma_k^2}} \frac{1}{\sqrt{1 - \gamma_k^2}} - \\ &\quad - \frac{\alpha^2 \beta}{zN} \sum_k \left(\frac{1}{\sqrt{1 - \gamma_k^2}} - 1 \right) \frac{1 - \sqrt{1 - \gamma_k^2}}{\alpha + \sqrt{1 - \gamma_k^2}} \quad (2) \end{aligned}$$

for ferromagnetic coupling, where $\langle S^z \rangle_{\text{And}}$ is the bulk sublattice magnetization [5] $\alpha = |I'/I|$, $\beta = S'/S$ and

$$\gamma_k = \frac{1}{z} \sum_\delta e^{ik\delta} \quad (3)$$

where the sum runs over the nearest neighbours.

Figures 1 and 2 show this modification of the zero-point spin contraction for bcc structure for five values of α . In this approximation this contribution is a linear

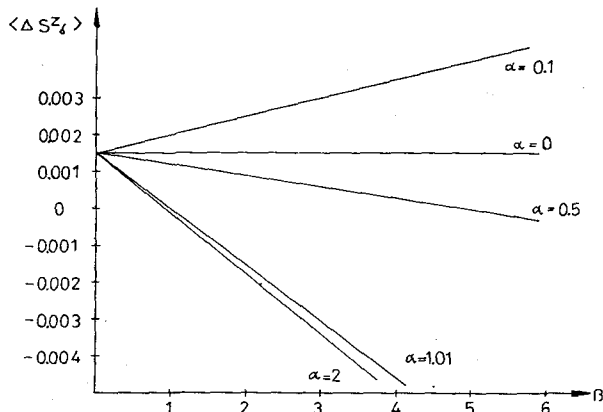


FIG. 1. — Change in the zero-point spin contraction on the first neighbours of an antiferromagnetically coupled impurity in bcc crystal.

function of β in contrast to Tonegawa's result [3], where for antiferromagnetic coupling an oscillating behaviour has been obtained. It is worth mentioning that in the special case, when $I' = 0$, the zero-point spin contraction on the first neighbours is smaller than that far from the impurity in agreement with van de Braak's [2] and Tonegawa's [3] result but in contradiction to that of Lovesey [1]. The absolute value of

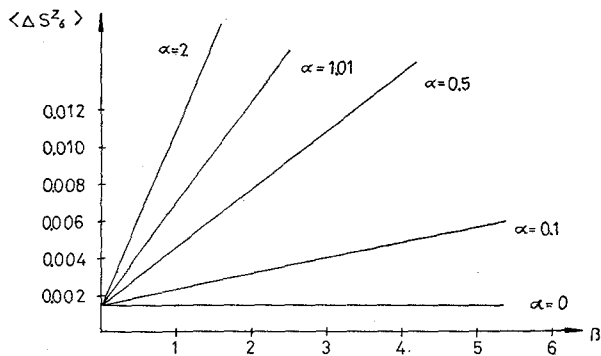


FIG. 2. — Change in the zero-point spin contraction on the first neighbours of a ferromagnetically coupled impurity in bcc crystal.

the reduction ($\langle \Delta S_z^2 \rangle = 0.0015$) is, however, smaller than that obtained by van de Braak.

For the impurity atom the first correction to the zero-point spin contraction appears already in first order in $1/z$. Instead of the lengthy formulae the result for antiferromagnetically and ferromagnetically coupled impurities in bcc crystal are given in figure 3 and 4. The non-linear behaviour is due to the second order

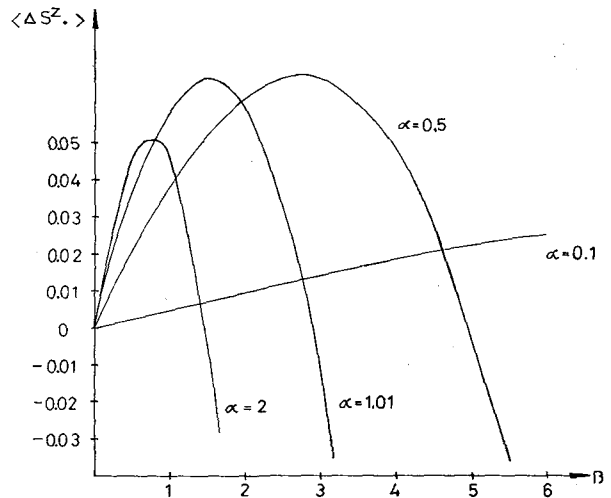


FIG. 3. — Zero-point spin contraction on an antiferromagnetically coupled impurity in bcc crystal.

terms. As it can be seen in figure 3 the approximation used breaks down with increasing value of α and β and only the initial slope can be taken seriously.

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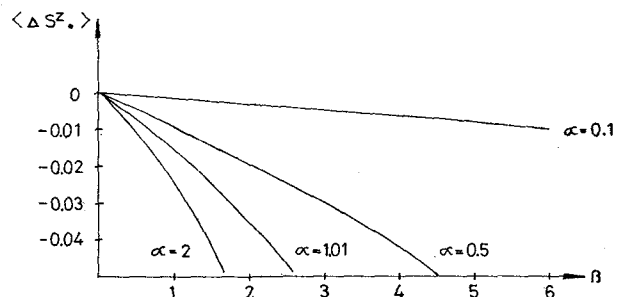


FIG. 4. — Zero-point spin contraction on a ferromagnetically coupled impurity in bcc crystal.

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