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ELECTRONIC ENERGY IN ITINERANT-ELECTRON METAMAGNETISM

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Electronic energy in the context of itinerant-electron metamagnetism is considered in a new way. In particular, the minimal value of this energy is calculated within the Stoner model. To get this end, an elliptic density of states is used.

1. INTRODUCTION

Itinerant-electron metamagnetism is a subject that has attracted some attention in recent years. However, the main problems related to this phenomenon remain unsolved from the theoretical point of view. Moreover, very little experimental work has been performed. Certainly, research work on itinerant-electron metamagnetism involves several difficult problems that must be solved before beginning the principal tasks. One of these problems deals with electronic energy when a magnetic field is acting on a given material. Magnetic field as well as temperature and pressure can be varied to produce a first-order transition between a non-magnetic state and a ferromagnetic one [1, 2]. This transition defines itinerant-electron metamagnetism.

In the following, we shall derive an approximate expression for the minimum value of the electronic energy in the previous context when a magnetic field is applied. This calculation will be performed for materials that exhibit the same Fermi level for the up and down spin bands. On the other hand, an elliptic density of states will be assumed in the context of the Stoner model [1, 2, 3]. Although this assumption is not entirely realistic, it gives rise to a model that agrees qualitatively with experiment [3, 4].

2. THEORY

According to the Stoner model, the electronic energy at T = 0°K is given by [2, 3]:

$$E_e = \int_{-W}^{E_{F1}} E\, g(E)dE + \int_{-W}^{E_{F2}} E\, g(E)dE - \frac{1}{4} JM^2 - \mu_B MH \qquad (1)$$

where 2W is bandwidth, E stands for energy, g(E) is the density of states, E_{F1} and E_{F2} are the Fermi levels of the up and down, respectively, J is the exchange energy between up and down spin electrons, μ_B is the Bohr magneton, M is the magnetization, and H denotes an applied magnetic field.

By introducing $E_{F1} \approx E_{F2}$ $(=E_F)$ in eq. (1) and using $g(E) \approx 3W^{-2}(W^2 - E^2)^{1/2}$ (see refs. [2, 3]), we shall minimize E_e. By imposing $(dE_e/dW) = 0$, we find, for a given M:

$$E_{e(min)} \approx -\left(\frac{1}{4} JM^2 + \mu_B MH\right) \tag{2}$$

On the other hand, we recall that the total energy is E_e plus the lattice energy E_l. Since E_l depends on volume variation, we can suppose that $E_l \ll E_e$ for transitions with very small volume change; denoted by E_t the total energy, we have $E_{t(min)} = E_{e(min)} + E_{l(min)}$. It has been derived $E_{l(min)} = 0$ (see ref. [3]); then $E_{t(min)} = E_{e(min)}$. In addition, we must take into consideration that W depends on volume. A formula to express this dependence has been given in ref. [3]; this expression was established in reality by Slater and Koster [5] by using a tight-binding approximation for 3d-electrons; the formula in question is [3, 5]:

$$W = W_0 \exp[\alpha(V_0 - V)/V_0] \tag{3}$$

where W_0 is the value of W for $V = V_0$ and α is a parameter such that $1 \leqslant \alpha \leqslant 5/3$. For $V - V_0 \ll V_0$, eq. (3) agrees with the Grado-Grado formula namely [2]:

$$W = \frac{W_0}{2}\left(5 - 3\frac{V}{V_0}\right) \tag{4}$$

3. CONCLUSIONS

We have found the minimum value of the electronic energy in the context of itinerant-electron metamagnetism. Although this result is not valid for intermetallic compounds, the theory exposed here agrees qualitatively with experimental data. Itinerant-electron metamagnetism has been observed in various rare-earth intermetallic compounds [6, 7]. In addition, we can mention vanadium oxide V_2O_3 in which a transition between the metallic phase and the antiferromagnetic insulating phase takes place with volume discontinuity [3, 8]. Finally, we can claim that the subjects treated here have some interest in several aspects of the electronic technology [2].

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