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Density of electron levels in ferromagnetic semiconductors

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The electron level density in a randomly oriented magnetic-moment field is considered. The optimal-fluctuation method is used to obtain an expression for the tail of the level density in wide-band ferromagnetic semiconductors at temperatures above the Curie point.

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1. INTRODUCTION

A characteristic feature of ferromagnetic semiconductors is the strong interaction of the conduction electrons with localized moments of the lattice magnetic atoms. Below the Curie point, the interaction of the electrons with the magnetic subsystem is described within the framework of the spin-wave approximation.[1] The long-range ferromagnetic order leads then simply to a shift of the bottom of the conduction band, without disturbing the translationally invariant system. In the paramagnetic region of temperatures, on the other hand, the magnetic order is disturbed, and the conduction electrons interact with the random field of the magnetic moments. This produces in the forbidden band a level-density tail due to exchange interaction of the electrons with the random vector field. The notion of a magnetic level-density tail has already been used a number of times to explain the optical and electrical properties of magnetic semiconductors at temperatures above the Curie point.[2]

In the present paper, using the optimal-fluctuation method, an expression is obtained within the framework of the single-electron approximation for the tail of the level density both for paramagnetic temperatures and for temperatures where the Ornstein-Zernike-Ginzburg-Landau expansion is valid.

2. PARAMAGNETIC TEMPERATURE REGION

In a ferromagnetic semiconductor, each crystal cell contains a rare-earth or transition element atom whose inner electron shell is only partly filled. The interaction of the conduction electron with the magnetic atoms is described by the s-d exchange Hamiltonian[1]

$$H_{s-d}=\frac{A}{2N}\sum_{g}(\mathbf{S}_g\mathbf{s})_{\sigma\sigma'}\Psi_\sigma^+(\mathbf{r})\Psi_{\sigma'}(\mathbf{r}), \tag{1}$$

where A is the s-d exchange constant, N is the number of atoms per unit volume, $\mathbf{S}_g$ is the spin of the magnetic atom, $\mathbf{s}$ is the spin of the conduction electron, $\Psi_\sigma^+(\mathbf{r})$ ($\Psi_{\sigma'}(\mathbf{r})$) is the operator of creation (annihilation) of an electron with spin $\sigma(\sigma')$ at the point $\mathbf{r}$. It is assumed that the width W of the conduction band is much larger than the s-d exchange energy AS, and furthermore $2S+1\gg 1$.

It is possible to separate in the Hamiltonian (1) components with diagonal ($\sigma=\sigma'$) and off-diagonal ($\sigma\neq\sigma'$) terms. The ratio of the contributions of the off-diagonal and diagonal terms is AS/W and will not be taken into account.

The starting point of the optimal-fluctuation method is a calculation of the probability of the fluctuation of a random quantity in a given spherical volume of radius R.[3] There are no known combinatorial formulas for the probability of the fluctuation of the magnetic moment produced in the region R by a random orientation of noninteracting spins. All that are available are some recurrence relations,[4] but their use calls for numerical methods.

In wide-band ferromagnetic semiconductors, where the parameter AS/W is small, a localized energy level is formed only by fluctuations whose radius is much larger than the lattice constant. To find the probability of their formation we can use the thermodynamic theory of fluctuations.[5] The probability P of the fluctuation of the moment M in a volume V and in the paramagnetic region of temperatures is given by

$$P\sim\exp[-M^2/2V\chi T]; \tag{2}$$

here χ is the magnetic susceptibility and T is the temperature. Reckoning the energy of the localized state down from the bottom of the conduction band, we express it in the form

$$-E=\frac{\hbar^2}{2mR^2}-\frac{AS}{2N_R}\frac{M}{\mu}, \tag{3}$$

where $N_R=V/a^3$ is the number of atoms in the volume, while a^3 and μ are the volume and the magnetic moment

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of the unit cell.

The first term in (3) corresponds to the kinetic energy of the electron, and the second to its exchange interaction with the fluctuation of the magnetic moment M. Just as when we restrict ourselves to spherical fluctuations, we lose here a numerical coefficient that depends on the true form of the wave function. With the aid of (3) we can represent the argument of the exponential (2) in the form

$$\frac{M^2}{2V\chi T}=\frac{2\pi\mu^2}{\chi T a^6}\left[\frac{1}{q_0^4R}+\frac{2}{q_0^2}\frac{E}{A}R+\frac{E^2}{A^2}R^3\right], \tag{4}$$

where $q_0^2=mAS/\hbar^2$. The radius R_0 of the optimal fluctuation, i.e., the radius at which (4) has a minimum, equals $R_0=q_0^{-1}(A/3E)^{1/2}$, from which we get for the level density the expression

$$\frac{\rho(E)}{\rho(0)}=\exp\left[-\frac{2\pi\mu^2}{\chi T a^3}\frac{1}{a^3q_0^3}\left(\frac{E}{A}\right)^{7/2}\right], \tag{5}$$

where $\rho(0)$ is the density of the electron levels at the boundary of the delocalized states.

3. ASYMPTOTIC LEVEL DENSITY WITH ALLOWANCE FOR CORRELATIONS

Formula (5) is valid for temperatures at which the size R_0, of the optimal fluctuation is large compared with the correlation radius R_c of the magnetic-moment correlations. If the condition $R_cq_0\ll 1$ is satisfied, then $R_0\gg R_c$ even for the maximal energies $E\sim AS$. On the other hand if $R_cq_0\gg 1$, then Eq. (5) is valid only at low energies for which $A/q_0R_cE\gg 1$. At $A/q_0R_cE\ll 1$, we obtain the optimal fluctuation by using the expansion of the Ornstein-Zernike thermodynamic potential Ω:

$$\Delta\Omega=\int\left[\frac{1}{2\chi}(\Delta\mathbf{M})^2+g\left(\frac{\partial\Delta\mathbf{M}}{\partial r}\right)^2\right]dV, \tag{6}$$

where $\Delta\mathbf{M}$ is the fluctuation of the magnetic-moment density, and g is a constant. The mean square fluctuation of the magnetic moment in a spherical region of radius R is defined with the aid of (6) as follows[5]:

$$\langle M^2\rangle_R=\frac{2\pi}{3}R^3\frac{T}{g}(R_c^2-RR_ce^{-R/R_c}-R_c^2e^{-R/R_c}), \tag{7}$$

where $R_c=(2g/\chi)^{1/2}$ is the correlation radius.

With the aid of (7) we can express the probability P of the magnetic-moment fluctuation in a spherical region of radius R in the form

$$P\sim\exp[-M^2/2\langle M^2\rangle_R]. \tag{8}$$

As $R_c\to 0$ Eq. (8) goes over into (2). If the radius of the optimal fluctuation is small compared with R_c, we can confine ourselves in the expansion $\langle M^2\rangle_R$ (7) to terms of second order in R/R_c. With the aid of (3) we can represent the argument of the exponential (8) in this case in the form

$$-\frac{M^2}{2\langle M^2\rangle_R}=-\frac{\pi gR}{3a^6T}\left(\frac{1}{q_0^2R^2}+\frac{E}{A}\right)^2. \tag{9}$$

The radius of the optimal fluctuation is here $q_0^{-1}(3A/E)^{1/2}$, and for the density of the electron levels we obtain the expression:

$$\frac{\rho(E)}{\rho(0)}=\exp\left[-\frac{\pi g}{T}\frac{1}{a^6q_0}\left(\frac{E}{A}\right)^{7/2}\right]. \tag{10}$$

The conditions for the applicability of formulas (5) and (10) are given respectively by the inequalities $(A/E)^{1/2}/q_0R_c\gg 1$ and $(A/E)^{1/2}/q_0R_c\ll 1$.

In this paper we have considered the influence of the field of random magnetic-moment orientations on the electron-level density. Formula (3) yields in the adiabatic approximation the energy of the interaction of the electron with the fluctuation of the magnetization for wideband ferromagnetic semiconductors, i.e., at $W\gg AS\gg T_C$, where T_C is the Curie temperature. The second term in (3) means that the spin of the conduction electron is directed along the summary moment produced by the random orientation of the spins of the magnetic atoms. A different situation arises in narrow-band magnetic semiconductors, where $W\ll AS$. The electron spin is directed here along the spin of the particular magnetic atom on which the electron is located.[6] The motion of the electron at $T>T_C$ is effected by jumping over to another magnetic atom having a spin orientation close to that of the initial atom. To find the level density in this case it is necessary to use the methods of percolation theory in a random spinor field. It is then also possible to use the adiabatic approximation, which is violated if the two inequalities $T_C\gg AS$ and $T_C\gg W$ are simultaneously satisfied.

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