# GROUND STATE AND ANOMALOUS MAGNETIC MOMENT OF CONDUCTION ELECTRONS IN AN ANTIFERROMAGNETIC SEMICONDUCTOR

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In considering the state of a conduction electron in an antiferromagnetic crystal it is customary to assume (cf. [1]) that it does not disturb the magnetic ordering of the crystal. It will be shown below that in many cases an energetically more favored state of the system is one in which the electron produces around itself a region with ferromagnetic ordering and moves together with this region through the crystal. In analogy with the polaron in ionic crystals [2], it is natural to call such a particle a magnetic polaron.

Within the framework of the s-d model, the state of the conduction electron + antiferromagnetic crystal system is determined essentially by three parameters: 1 - the integral A of exchange interaction of the conduction electron with the d-electron of the magnetic atom nearest to it, 2 - the Bloch integral B, to which the width of the conduction electron band is proportional in the absence of exchange with the d-electrons, and 3 - the exchange integral I for the neighboring magnetic atoms. It is essential that the last of these parameters is small compared with the other two: A and B are of the order of 0.1 - 1 eV, and I is of the order of 0.01 or even 0.001 eV.

If we assume that the antiferromagnetic ordering remains unchanged, then the energy of the s-electron, neglecting the zero-point oscillations of the sublattice magnetic moments, is given by the expression

$$E_{e0} = E_A - \sqrt{z^2 B_k^2 + \frac{1}{4} S^2 A^2}, \qquad (1)$$

$$B_k = 2B[\cos k_x a + \cos k_y a + \cos k_z a],$$

where $E_Z$ is the "atomic" energy of the s-electron, S the spin of the magnetic atom, z the number of nearest neighbors, and a the lattice constant.

As is well known, the translational motion of the electron over the crystal leads to a lowering of its ground state. It is seen from (1) that when $z|B| \ll S|A|$ the antiferromagnetic ordering hinders the translational motion of the conduction electron in the crystal. In the opposite limiting case it leads to an appreciable decrease in the role of s-d exchange. But if we assume that the conduction electron produces around itself a region of ferromagnetic ordering, then it becomes possible to obtain enhancement of the electron energy as a result of its translational motion in this region, or exchange with magnetic atoms in this region. This enhancement offsets the energy loss due to the disturbance of the antiferromagnetic ordering. The radius of the ferromagnetic potential well is obtained from the condition that the total energy of the system be minimal.

We confine ourselves here to consideration of a magnetic polaron at rest. The system energy is obtained from a variational principle. When $A > 0$, the trial function of the system is chosen in the following fashion: 1 - the polarization of the conduction-electron spin

is fixed (the spin is parallel to the moment of the ferromagnetic well). 2 - The state of the magnetic subsystem does not depend on the position of the conduction electron. At r = R the ideal antiferromagnetic ordering (r > R) goes over jumpwise into ideal antiferromagnetic ordering (r < R). 3 - The electronic part of the trial function is constructed as a linear combination of s-orbits corresponding to different magnetic atoms. Its coefficients $\psi(g)$ (g is the number of the magnetic atom) are determined from the equation

$$[E_A - \frac{A}{2} < S_g^z > - E]\,\psi(g) + B \sum_h{}' \psi(g+h) = 0. \tag{2}$$

The prime at the summation sign in (2) denotes summation over the nearest neighbors, and <...> is the averaging symbol.

It is convenient to represent the function $\psi(g)$, defined at all lattice points, as a spinor whose components $\psi_i$ (i = 1, 2) are defined only at those sites which whould form the i-th magnetic sublattice. The radius of the magnetic polaron amounts in typical cases to several lattice constants. It is therefore advantageous to go over to the approximation of a continuous medium, expanding the last term of (2) in a Taylor series about the point g and considering the coordinates of the lattice sites as continuous variables. Taking the statements mad above with respect to the state of the magnetic subsystem into account, we obtain the following set of equations:

$$\begin{gathered}
\{E_A - \frac{AS}{2} - E\}\,\psi_1(r) + B[z + a^2\Delta]\,\psi_2(r) = 0\,, \\
B[z + a^2\Delta]\,\psi_1(r) + \{E_A + \frac{AS}{2}[1 - 2\theta(R-r)] - E\}\,\psi_2(r) = 0\,, \\
\theta(x) = 1 \text{ if } x > 0 \text{ and } = 0 \text{ if } x < 0.
\end{gathered} \tag{3}$$

Solution of the system (3) leads to the following expression for the energy

$$\begin{gathered}
E = E_n + \frac{4\pi}{3}\frac{R^3}{a^3}\,|I|\,S^2 z, \\
E_n = E_A - \frac{AS}{2} - |B|\,[z - k^2 a^2],
\end{gathered} \tag{4}$$

where the parameter k is given by the equation

$$\begin{gathered}
k^2 a^2 = (z - k^2 a^2)\,[\sqrt{1 + \frac{AS}{|B|\,(z - k^2 a^2)}} - 1]\,\sin^2 kR \\
(\frac{\pi}{2} \leqslant kR \leqslant \pi).
\end{gathered} \tag{5}$$

According to (4) and (5), the energy $E_n$ of the electron captured by the magnetic polarization assumes, as a function of R, values from a maximum coinciding with the bottom of the conduction band of the free electron in an ideal antiferromagnet (1) to a minimum equal to

$$E_A - \frac{AS}{2} - z|B|.$$

At parameter values for which the minimum of the total magnetic-polaron energy is reached

in the region where the continual theory is valid, the order of magnitude of R is $a(B/|I|S^2z)^{1/5}$.

It should be noted that when S and R are small it is necessary to take into account the fluctuations of the conduction-electron spin outside the ferromagnetic region. The appropriate calculations will be reported in a separate article.

The foregoing analysis can be extended to include the case $A < 0$, by replacing A with $|A|$, if $|A/B|$ is sufficiently small. In the opposite case, the s-electron spin cannot be regarded as fixed, and the wave function takes into account the oscillations of the d-electron spins in the ferromagnetic well, owing to their exchange with the s-electron. We then get

$$E_n \simeq E_A - \frac{1}{2}|A|(S+1) - |B|\left(\frac{2S}{1+2S}\right)\left[z - \frac{\pi^2 a^2}{R^2}\right]. \qquad (6)$$

As seen from (6), the second variant of the trial function, which ensures, unlike the first, a full gain of the s-d exchange energy, results at the same time in some loss of translation-energy motion.

A characteristic feature of the magnetic polaron is its anomalously large magnetic moment, which can exceed 100 Bohr magnetons. This moment should affect particularly storngly the longitudinal magnetic susceptibility of the antiferromagnet. An anomalous moment should also be possessed by the electron captured by the impurity center, but its value is smaller than that of the free magnetic polaron. Thermal ionization of the impurity centers should therefore lead to an increase of $\chi$ until the magnetic polarons begin to dissociate. At high densities of the alloying impurity, the increase of temperature can lead in principle to a transformation of the crystal into a ferromagnetic one with a simultaneous sharp increase of the electric conductivity.

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[1] Yu. P.Irkhin and E. A. Turov, FMM 4, 9 (1957)
[2] S. I. Pekar. Issledovaniya po elektronnoi teorii kristallov (Research in the Electron Theory of Crystals), GITTL, 1951; S. V. Tyablikov, JETP 21, 377 (1951).

## SELF-FOCUSING OF LIGHT IN SOLIDS VIA THE ELECTROSTRICTION MECHANISM

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The self-focusing of light is dealt with in [1-3]. The structure of the light beam in the case of self-focusing by electrostriction was investigated in detail in [3]. It will be shown here, however, that the results of [3] are not applicable even in an isotropic solid, and pertain only to a liquid. The point is that a deformation that is uneven over the volume of a solid, and the corresponding change in the refractive index, cannot be connected with only the local value of the electrostriction force, as is done in [3]. An investigation shows that if the self-focusing mechanism via electrostriction does exist in solids, then the beam in the channel will have a rather complicated polarization.

We consider for simplicity stationary self-focusing of unpolarized light in an isotropic