Ferron mechanism of charge transport in antiferromagnetic semiconductors and its peculiarities at phase separation

E. L Nagaev

Institute for High Pressure Physics of Russian Academy of Sciences

The energy spectrum of moving one- and many-electron ferrons is investigated (the ferron is a carrier self-trapped in a ferromagnetic microregion of an antiferromagnetic semiconductor). The ferron band width decreases exponentially with increase of the ferron radius. On increase of number of electrons in a many-electron ferron, its effective mass reduces at first, and then, after passing through a minimum, sharply increases. In imperfect crystals the ferron motion occurs via phonon-assisted random walks of which the probability decreases exponentially on increase in the ferron radius. Experimental data[8] on the high-field conductivity are analyzed for heavily-doped EuTe in the state when it is separated into the insulating antiferromagnetic and high-conductivity ferromagnetic phases, the latter consisting of many-electron-ferrons forming an almost periodical structure. Electric fields high enough cause depinning of ferrons and current pulsations arise.

INTRODUCTION

The concept of ferrons in an antiferromagnetic semiconductor was advanced by the author of the present publication as far back as 25 years ago:[1] it was proved that the conduction electron (or a hole) may create a ferromagnetic region inside the antiferromagnetic structure and stabilize this region by localization of this charge carrier in it. Thereafter a very large literature was devoted to the ferron (some authors call it magnetic polaron or spin-polaron, see the mohograph[2] and the latest review article[3]). Experimentally, ferrons were first discovered in EuTe and EuSe.[4]

The one-electron ferrons mentioned above are typical of nondegenerate semiconductors. In degenerate antiferromagnetic semiconductors many-electron ferrons may arise when there are several conduction electrons in the same ferromagnetic region. Sometimes the number of these electrons may be very large. The crystal turns then, out to be separated into antiferromagnetic and ferromagnetic phases, with all the conduction electrons concentrated in the latter and with the former being insulating. Phase separation in degenerate antiferromagnetic semiconductors, the idea of which was advanced and a detailed investigation was carried out in the present author's papers[5] 20 years ago, has become very popular with investigators quite recently because it is supposed to be related to the high-temperature superconductivity. Unfortunately, my results[5] remained unknown to authors of subsequent papers on the phase separation, and they were unable even to reproduce results. Experimentally, the antiferromagnetic-ferromagnetic two-phase state was observed in degenerate antiferromagnetic crystals EuTe and EuSe.[6,7]

Practically in all the papers on ferrons it was assumed that their effective mass was infinitely large, so that they cannot take part in the charge transport. Such an approach is quite satisfactory in many cases. For example, transition of the photoelectrons, generated by illumination, into ferron states sharply reduces the photoconductivity of EuTe and EuSe crystals. This means that the ferron contribution to the electrical current is negligibly small compared with photoelectrons. As to degenerate antiferromagnetic semiconductors, according to Ref. 5, at not too high carrier densities, the high-conductivity regions of the ferromagnetic phase form a periodic structure inside the insulating antiferromagnetic host. Each conduction electron is locked inside its ferromagnetic droplet and cannot move throughout the entire crystal. For this reason, if the ferromagnetic high-conductivity droplets are stationary the degenerate semiconductor should display insulating properties. Transition of degenerate antiferromagnetic semiconductors into an insulating state, accompanied by appearance of magnetized regions inside them, was observed experimentally on decrease in temperature.[6,7]

It should be noted that, nevertheless, experimental data just described do not exclude the possibility of situations in which the charge transport by the ferrons may play a basically important role though their mobility is extremely low. Strictly speaking, if the crystals had been ideal, the ferrons in degenerate semiconductors would have moved under an arbitrarily small electric field. Their immovability may be explained by their pinning due to the electrostatic-potential fluctuations of the impurity, introduced into the crystal to produce free charge carriers. This phenomenon strongly resembles pinning of the charge density waves in systems where they realize. As well known, in strong external electric fields depinning of CDWs occurs, and charge transport by them begins which leads to a nonlinear current-voltage characteristic (IVC) of such systems. It seems natural to believe that a strong electric field applied to antiferromagnetic semiconductors may cause depinning of ferrons.

Though the ferronic charge transport, like the CDW transport, is of cooperative type, response of the ferron system to the external electric field should be quite different than that of the CDW system. As was already mentioned, in the zeroth approximation in the impurity-

potential fluctuations, the ferromagnetic droplets form a periodic structure. Hence, when the ferromagnetic droplets move in an external electric field, their layers reach the cathode simultaneously, and at that moment the current flash occurs. After this the current vanishes, and it reappears when the next layer of ferromagnetic droplets reaches the cathode, and so on. Obviously, the pulse spacing is the less, the more rapidly the droplets move, i.e., the larger the external field. Thus, in the case under consideration, a strong constant field should cause a pulsed current of which the frequency increases with the field strength.

This theoretical prediction agrees with recent experimental data obtained for heavily doped EuTe which behaves above 170 K like a conventional degenerate semiconductor and below 170 K goes over into a state of very low conductivity. If one applies a rectangular potential pulse, then at not very high field strengths the response of the system duplicates the shape of the pulse. This can be naturally related to the charge transport by free carriers, a relatively small number of which is always present in the sample. But, beginning with a certain threshold potential, narrow current peaks appear on the background of the rectangular current pulse. Their height is several factors of ten larger than the height of the rectangular current pulse. The peak spacing decreases with increasing field strength.

Before we conclude that the current pulsations in Ref. 8 are due to the motion of the ferromagnetic droplet layers, we must assess other possible explanations of this effect. As is well known, current pulsations may be caused by high- and low-field domains formed in nondegenerate semiconductors with N-shaped IVC.[9] As applied to the situation considered, it should mean that the ferromagnetic droplets remain stationary in the external field, but the field causes separation of the free charge carrier heated by it, into moving domains of the high- and low field. A current pulse arises when a domain with enhanced density of free carriers passes through the cathode. But the current drops sharply when this domain becomes replaced by a domain with a reduced carrier density.

But the fact that the rectangular current pulse retains its height unchanged in Ref. 8, and the current spikes do not alternate with its dips is evidence that the domains of hot free carriers are absent from EuTe. Consequently, the current spikes may be explained by superposition of the current due to the free conduction electrons and the current due to the many-electron ferrons. The explanation of the effect, proposed by the authors of Ref. 8 themselves, according to which the hot electrons destroy ferrons and liberate electrons previously localized inside them, which then cool down and form the ferrons again, is more readily heuristic. In fact, they regarded the current spike as a result of the Auger process which, as well known, leads not to an N-shaped but to an S-shaped IVC.[9]

It should, nevertheless, be noted that, in principle, an N-shaped IVC can be realized in degenerate semiconductors in a two-phase antiferromagnetic-ferromagnetic state. Though there is no evidence that the Gunn effect related to the additional minimum in the conduction band is possible in them, an N-shaped IVC may result from the Coulomb barrier for the recombination processes.[9] In fact, from the point of view of semiconductor physics, each ferromagnetic droplet plays the part of a multiply-ionized impurity center. Being occupied by several electrons simultaneouly, the ferromagnetic region repels the electron that had left it for the conduction band. To return to this region by recombination, the electron must overcome this repulsion, and heating by the electric field favors it. N-shaped IVC are well known for nonmagnetic semiconductors with impurity centers.

Beside transport phenomena in strong electric fields, there is another reason which makes the problem of ferron motion vital: their possible role in the high-temperature superconductivity (HTSC). Attention to it was first drawn in Ref. 10, where it was proposed that ferron pairing can lead to HTSC. According to Ref. 10, ferron pairing leads to formation of Bose quasiparticles (biferrons) which may play the part of the Cooper pairs. Although such an HTSC mechanism, is certainly hypothetical, there are no reasons to declare it impossible at all. The fact that the Hubbard model in which the ferron is unstable[2,11] is used in Ref. 10 does not cast any doubts on the basic idea of Ref. 10, though one should deal with expressions presented there with care, the more since they are given without derivation.

Since for reasons mentioned above the problem of the moving ferron is timely now, this paper is devoted to investigation of the ferron dispersion law in ideally periodical crystal at $T=0$. The ferron effective mass will be found as a function of the ferron size, number of electrons in it, and magnitude of the magnetic atom spins. Knowledge of the ferron effective mass makes it possible to draw important conclusions concerning its kinetics. In imperfect crystal the ferron moves not according to the band mechanism but via random walks. It will be investigated, too, but at finite temperatures.

It should be indicated that the problem of the ferron effective mass is much more complicated than the same problem for the Pekar polaron, which like the ferron is a self-trapped state of the charge carrier. The reason for it is the fact that the interaction of the conduction electron with optical phonons is linear whereas its interaction with the magnetic subsystem in an antiferromagnetic crystal is essentially nonlinear. Thus, the elegant Pekar's approach to the problem of the polaron effective mass cannot be used here.

In view of its complexity of the problem, the analysis is confined on a one-dimensional model. It is shown that the ferron motion throughout the crystal is mainly caused by a specific indirect exchange interaction between magnetic atoms via the electron (or electrons) localized inside the ferron. On increase in the ferron radius, the width of its energy band decreases exponentially. On increase in the number of electrons in a many-electron ferron, the width of its band increases at first, and then, after passing through a maximum, falls off very sharply. A rather unexpected conclusion follows from these results: increase in the number of charge carriers in the crystal may not only increase but also decrease the ferron conductivity. The origin is the fact

that both the ferron radius and number of electrons in it increase with the charge-carrier density.

The estimates for the ferron effective mass obtained here correspond to values of the order of the ion mass. The width of the ferron band is so small that in real imperfect crystals the Anderson localization of ferrons should take place, i.e., their spontaneous motion throughout the crystal is impossible. But strong electric fields liberating ferrons from their potential wells make it possible for them to move. Their movement is the more rapid, the less is their effective mass. At temperatures high enough even in an ideal crystal the ferron motion occurs via random walks accompanied with ferron shape fluctuations.

MODEL

To clarify the qualitative peculiarities of ferron motion and obtain the necessary estimates, we consider below the geometrically simplest one-dimensional crystal model. The calculation will be carried out within the framework of s–f (or, equivalently, s–d) model, of which a particular case is in fact the now very popular t–I model. The system Hamiltonian is written in the form

$$H = H_0 + H_1 + H_2,$$

$$H_0 = B \sum a^*_{g,\sigma} a_{g\pm1,\sigma} - A \sum \sigma S^z_g a^*_{g,\sigma} a_{g,\sigma} - \lambda I \sum S^z_g S^z_{g+1},$$

$$(1)$$

$$H_1 = -A \sum (\mathbf{s}, \mathbf{S}_g)_{\sigma,-\sigma} a^*_{g,\sigma} a_{g,-\sigma},$$

$$H_2 = -I \sum (S^+_g S^-_{g+1} + S^-_g S^+_{g+1}), \quad (S^\pm = S^x \pm iS^y),$$

where $\mathbf{S}_g$ is the operator of the f-spin of the atom g, $a^*_{g,\sigma}$, and $a_{g,\sigma}$ are the operators of creation and annihilation of an s-electron with spin projection σ on the atom g, and $\mathbf{s}_{\sigma\sigma'}$ are Pauli matrices. According to the physical meaning of the problem, the integral I of the direct f–f-exchange is assumed to be negative. The signs of other parameters are inessential. For the sake of definiteness, the Bloch integral B will be assumed negative and the s–f-exchange integral A positive.

As is known, in one-dimensional Heisenberg systems the role of zero-point spin fluctuations is so large, that the classical picture of the antiferromagnetic ordering becomes generally speaking inadequate. To justify, as in many-dimensional cases, the use of the classical picture of an antiferromagnet as the zeroth approximation of the true state of the magnetic subsystem, the direct f–f- exchange is assumed to be anisotropic with the anisotropy parameter λ exceeding unity.

To model the rare-earth compounds, we assume that the ratio AS/W is the small parameter of the problem. Here $W = 4|B|$ is the conduction-band width and S the magnitude of the f-spin.[2] In addition, the obvious inequality $AS \gg IS^2$ is assumed met.

At first the case $S = 1/2$ will be discussed. Then the zeroth-approximation Hamiltonian H_0 can be diagonalized exactly, making it possible to find the ground-state energy

for the system "conduction electron + antiferromagnetic crystal." With favorable parameter relations this state corresponds to a stationary ferron, when in a portion of the one-dimensional crystal of length $2R$ the antiferromagnetic ordering is replaced by the ferromagnetic. This portion is the potential well of depth $U = AS/2$ for the conduction electron. According to the condition $W \gg AS$, bound states exist in it only if R is large enough. Since the electron levels in a shallow potential well are also shallow, the effective-mass approximation is valid for their description. The radius R should be found from the condition that the total energy of the system is a minimum.

At very large sizes of the ferromagnetic region, the ferron energy is given by the expression

$$E_F = |I|R/a + \pi^2/2mR^2 - A/4,$$

$$1/m = 2|B|a^2 \quad (\hbar = 1),$$

$$(2)$$

where a is the lattice constant. As follows from (2), the equilibrium value of the radius R is given by the expression

$$R = |\pi^2 a/mI|^{1/3} \sim |B/I|^{1/3} \tag{3}$$

and the ferron can exist if

$$|I|^{2/3}|B|^{1/3} < A \tag{4}$$

(the last condition can be obtained also by a more rigorous analysis).

The motion of the ferron throughout the crystal is the result of action of the transverse components of the Hamiltonians H_1 and H_2, describing the the s–f and f–f exchange. The Hamiltonian H_2 directly changes the f-spin configuration, and the conduction electron follows the magnetic subsystem adiabatically. The Hamiltonian H_1 does the same by means of indirect exchange between the f-spins via the s-electron localized in the ferromagnetic region. In this case the ferron motion over the crystal is initiated by the electron localized inside the ferron. But one cannot use the continuum approximation to describe the ferron motion, since the problem is nonlinear. For this reason our treatment will be microscopic.

First of all, it should be pointed out that, strictly speaking, two types of the ferron states are possible, and are both eigenstates of the Hamiltonian H_0: 1) the central atom of the ferron belongs to the antiferromagnet sublattice in which the directions of the f-spins remain unchanged by ferron formation; 2) the central atom belongs to the other sublattice whose f-spins are reversed inside the ferromagnetic region.

Though for large radii R the energies of these two states are close to each other, different projections of the total spin of the system correspond to them, since in the first case an even number of f-spins is reversed upon ferron formation, whereas in the second case this number is odd. Since the Hamiltonian H (1) conserves the total spin projection of the system, it cannot transform a ferron of the first kind into a ferron of the second type. Hence, the translation of the ferron over the crystal cannot amount to one lattice constant. The minimum translation should amount to two lattice constants, so that the center of the ferron

belongs to the one and the same sublattice despite the translational motion of the ferron. This means that the ferron is characterized not by the crystallographic but by the magnetic translational symmetry.

In what follows, the first case will be considered for definiteness. The treatment that follows can be easily generalized for the second case. The number of the atom coinciding with the ferron center is denoted by $2l$, and the boundary atoms of the ferromagnetic region have the numbers $2l \pm r$ ($r=R/a$ where a is the lattice constant). Obviously, they belong to the same sublattice as the central atom, i.e., their spins are not reversed.

The wave function of the magnetic subsystem for such a configuration may be presented in the form

$$\varphi_{2l}= \prod_g \delta(S^z_{2g+1},M_{2g+1-2l}) \prod_f \delta(S^z_{2f},1/2), \qquad (5)$$

where the quantity $M_{2g+1-2l}$ is equal to $1/2$ inside the interval $|2g+1-2l| < R$ and to $-1/2$ outside this interval, $\delta(n,m)$ is a delta-function of a discrete argument.

The electron part of the Hamiltonian H_0, corresponding to the spin configuration (5), is diagonalized by the canonical transformation of the electron operators

$$a_{2l,i,1/2}= \sum_h \alpha_i(h-2l)a_{h,1/2} \qquad (6)$$

yielding the electron spectrum $E_{i,1/2}$, where the quantum number i denotes the number of the discrete level inside the potential well or the electron momentum outside it. Thus, if the one-electron ferron is energywise favored, the eigenfunctions of the ground state for the Hamiltonian H_0 are given by the expressions

$$\psi_{2l}=\alpha_{2l,0}\Phi_{2l}, \quad \alpha_{2l,0}=a^*_{2l,0,1/2}|0\rangle \qquad (7)$$

where $|0\rangle$ is the vacuum s-electron wave function.

ONE-ELECTRON FERRON MOTION CAUSED BY THE DIRECT EXCHANGE

Qualitatively, the ferron motion, caused by the direct-exchange Hamiltonian H_2 taken in the first-nearest-neighbor approximation occurs in the following manner. According to (5) the ferron moment is directed upwards. In the first stage, reversal from up to down of the spin of a boundary atom (e.g., with the number $2l+r$) takes place with simultaneous reversal, in the opposite direction, of the spin of its nearest neighbor outside the ferromagnetic region with the number $2l+r+1$ which becomes directed upward. With allowance for the fact that the spin of the atom $2l+r+2$ is also directed upwards, i.e., parallel to the magnetic moment of the ferron, the right-hand boundary of the ferromagnetic region reaches this atom but, on the other hand, inside this region the spin $2l+r$ appears with the direction opposite to its moment. This irregular spin goes over from the atom $2l+r$ to its left neighbor $2l+r-1$, from it to the atom $2l+r-2$, and so on, until it reaches the atom $2l-r+1$. It turns out at that instant that the completely ferromagnetic region is enclosed between the atoms $2l-r+2$ and $2l+r+2$ without down spins inside it. This means that the ferron is displaced two lattice constants to

the right and its center is located at the atom $2l+2$. The picture described reveals that the ferron motion can be regarded as a result of motion of a magnon inside the ferron in a direction opposite to the direction of the ferron motion.

To describe the spin-wave motion to which the electron of the ferron adjusts itself, the wave functions $\beta_{2l+1,n}$ are introduced. Being the eigenfunctions of the Hamiltonian H_0, they correspond to excited states of the magnetic subsystem. Namely, they describe the ground state of the s-electron when the ferromagnetic region is bounded by the atoms $2l-r$ and $2l+r-2$, but at the distance n from the central atom $2l+1$ spin of the atom is antiparallel to the ferron moment. The state of the ferron is described in this case by the wave function

$$\widetilde{\psi}_{2l+1,n}=\beta_{2l+1,n}\widetilde{\Phi}_{2l+1,n},$$

$$\beta_{2l+1,n}= \sum_g \beta(g-2l-1,n)a^*_{g,1/2}|0\rangle \qquad (8)$$

$$\widetilde{\Phi}_{2l+1,n}=S^+_{2l+r+1}S^-_{2l+1+n}\Phi_{2l}.$$

With allowance for equalities

$$\Phi_{2l+2}=S^+_{2l+r+1} S^-_{2l-r+1} \Phi \quad \text{and} \quad \Phi_{2l-2}$$

$$=S^+_{2l-r-1} S^-_{2l+r-1}\Phi_{2l}$$

one obtains formally:

$$\widetilde{\psi}_{2l+1,-r}=\widetilde{\psi}_{2l-1,r}=\psi_{2l+2}; \quad \widetilde{\psi}_{2l+1,r}=\widetilde{\psi}_{2l-1,-r}=\psi_{2l}.$$

The wave function of the moving ferron is sought in the form

$$\psi= \sum x_{2l}\psi_{2l}+ \sum y_{2l+1,n}\widetilde{\psi}_{2l+1,n}. \qquad (9)$$

Then in the first order in A/W the spectrum of the moving ferron is found from the set of equations that follows from (1), (7), (8), and (9) (the energy is reckoned from the energy of the stationary ferron):

$$Ex_{2l}= -(I/2)[y_{2l+1,r-1}$$

$$\times (\alpha_{2l,0},\beta_{2l+1,r-1})$$

$$+y_{2l-1,-r+1}(\alpha_{2l,0},\beta_{2l+1,-r+1}),$$

$$[E-(A/4)\beta^2_{2l+1,n}-\lambda I]y_{2l+1,n}$$

$$= -(I/2) \sum_{(\pm)} y_{2l+1,n\pm 1}(\beta_{2l+1,n},\beta_{2l+1,n\pm1}),$$

$$[E-(A/4)\beta^2_{2l\pm1,\pm(r-1)}-\lambda I)y_{2l\pm1,\pm(r-1)}$$

$$= -(I/2)[y_{2l\pm1,\pm(r-2)}(\beta_{2l\pm1,\pm(r-1)},\beta_{2l\pm1,\pm(r-2)})$$

$$+x_{2l}(\beta_{2l\pm1,\pm(r-1)},\alpha_{2l,0}). \qquad (10)$$

In what follows, in the leading order in Ia/AR, one may put all the scalar products of the electron wave functions in (10) equal to unity. To obtain a semiqualitative solution of the set of equations (10) one may set all the diagonal matrix elements equal to their average values:

$$-(A/4)\beta_{2l+1,n}^2 - \lambda I \to -A/8R - \lambda I \equiv \chi I. \qquad (11)$$

Then with allowance for the translational symmetry of the system the coefficients of the expansion (9) may be sought in the form

$$x_{2l} = X\exp(i2pl);$$

$$y_{2l+1,n} = \{Y\exp(qn) + Y^*\exp(-qn)\} \qquad (12)$$

$$\times \exp[i(2l+1)p].$$

Substitution of Eqs (11) and (12) in (10) leads to the following dispersion relation for the ferron:

$$\varepsilon = -(2E/I - 2\chi) = 2\,\mathrm{ch}\,q,$$

$$\mathrm{ch}\,q + \chi = \mathrm{ch}\,q(r-1) \qquad (13)$$

$$\times \cos^2 p/\mathrm{ch}\,rq + \mathrm{sh}\,q(r-1)\sin^2 p/\mathrm{sh}\,qr.$$

Its solution putting $q = i\pi + x$ yields an expression for the ferron dispersion law (its quasimomentum p is assumed to be dimensionless):

$$E(p) = |I|\,[\chi - (1+\chi^2)^{1/2} + \chi(1+\chi^2)^{-1/2}$$

$$\times (\chi + \sqrt{1+\chi^2})^{-2r}\cos 2p]. \qquad (14)$$

As follows from (14) the direct exchange leads to broadening of the ferron level into a band whose width is exponentially small compared to the magnon bandwidth $\sim I$, and decreases sharply with increasing radius R.

FERRON MOTION DUE TO INDIRECT EXCHANGE

If the direct exchange is weak, a much more powerful mechanism causing motion of the ferron is indirect exchange via the electron of the ferron. Unlike the indirect exchange in rare-earth metals, one cannot describe this kind of interaction between f-spins in terms of an effective Hamiltonian, since the magnetic properties of the system are nonanalytic in the s–f exchange integral, as a consequence of the complete spin polarization of the s-electron.[2] For this reason, as before, the variational procedure will be used, but additional account will be taken here of the virtual states with the reversed spin of the s-electron, states that arise as a result of the f-spin reversal of the magnetic atom adjacent to the ferron boundary. Such virtual states are described by the wave functions

$$\widetilde{\widetilde{\psi}}_{2l+1,k} = \gamma_{2l+1,k}S_{2l+r+1}^+\Phi_{2l}, \qquad (15)$$

$$\gamma_{2l+1,k} = \sum \gamma_k(g-2l-1)a_{g,-1/2}^*|0\rangle,$$

where k is the index of the electron state. In the zeroth approximation in AS/W the electron wave function is simply a plane wave, and the index k is its wave number.

Correspondingly, the trial wave function of the ferron is sought in the form that allows spin reversals for pairs of atoms, both at the opposite boundaries of the ferromagnetic region and at one of boundaries and inside the region:

$$\psi = \sum x_{2l}\psi_{2l} + \sum y_{2l+1,n}\widetilde{\psi}_{2l+1,n} + \sum z_{2l+1,k}\widetilde{\widetilde{\psi}}_{2l+1,k}. \qquad (16)$$

The wave function (16) makes it possible to describe both the direct transfer of a spin projection from one boundary atom to the other and the indirect transfer via a magnon propagating through the ferromagnetic region. The latter mechanism resembles the mechanism discussed in the preceding section but here the spin can jump over several lattice constants.

A system corresponding to (10) should be supplemented in this case with equations with respect to $z_{2l+1,k}$. In the set of equations obtained in such a way, one may omit the direct-exchange integral at small I since the mean indirect-exchange energy A/R is according to (3) of the order of $A|I/W|^{1/3}$ and therefore certainly exceeds the direct-exchange energy I.

After eliminating the coefficients $z_{2l+1,k}$ from this set of equations, it acquires the indirect-exchange integrals

$$J(n-n') \simeq (A^2/4)\sum \gamma_k^*(n)\gamma_k(n')[k^2/2m + A/2]^{-1}$$

$$= (maA^2/4x)\exp\{-x|n-n'|a\},$$

$$x = (mA/2)^{1/2}. \qquad (17)$$

Attention should be called to the fact that the indirect-exchange integral (17) diminishes with increasing interatomic distance according to an exponential law and not in the oscillatory fashion as in the RKKY theory. Nevertheless, with allowance for the condition $W \gg A$ the decay length for the indirect exchange $1/x$ should considerably exceed the lattice constant. This is a direct consequence of the fact that the minimum energy of an electron with the spin $1/2$ is lower by $\sim A/2$ than the energy band of an electron with spin $(-1/2)$. Correspondingly, the indirect-exchange integral turns out to be nonanalytic in A, as manifested by the parameter x. It is worth mentioning that the indirect-exchange integral in degenerate ferromagnetic semiconductors possesses a structure similar to (17) and related to the complete spin-polarization of the conduction electrons. It is just by this structure that the symmetry property of an isotropic ferromagnetic structure, the gapless magnon spectrum, is manifested.[2]

A set of equations similar to (10), obtained in the manner just mentioned, takes the form

$$[E + 2\alpha^2(r+1)J(0)]x_{2l} = -\alpha^2(r+1)J(2r)$$

$$\times (x_{2l+2} + x_{2l-2}) - \alpha(r+1)$$

$$\times \sum_n \beta(n,n)[J(r-n)y_{2l+1,n}$$

$$+ J(r+n)y_{2l-1,n}]; \qquad (18)$$

$$[E-A\beta^2(n,n)/2]y_{2l+1,n}=-\beta(n,n)\Big|\alpha(r+1)[J(r-n)$$

$$\times x_{2l}+J(n+r)x_{2l+2}]-\sum_{n'}$$

$$\times J(n-n')\beta(n',n')y_{2l+1,n'}\Big|,$$

$$\alpha(n)\equiv\alpha_0(n) \qquad (19)$$

(the nonorthogonality integrals for the electron wave functions in the main approximation in a/R are put equal to 1).

To obtain an approximate solution of the set of equations (18), (19) it should be noted that the typical length over which the coefficient $y_{2l+1,n}$ changes as a function of n should be the same as for the exchange integral $J(n)$. This makes it possible to put $y_{2l+1,n'}\approx y_{2l+1,n}$ in the last term in (19) under the summation sign. Then the approximate solution of the integral equation (19) may be approximated by

$$y_{2l+1,n}\approx\beta(n,n)\alpha(r+1)[J(r-n)x_{2l}+J(r+n)x_{2l+2}]$$

$$\times[E-K\beta^2(n,n)]^{-1}, \qquad (20)$$

$$K=A/2+mA^2/2(\varkappa^2+\pi^2/4R^2)$$

To obtain (20) the fact was used that in the main approximation in A/W the wave function $\beta(n,n)$ is of the form

$$\beta(n,n)=(r+1)^{-1/2}\cos qn,$$

$$q=[\pi/2(r+1)][1-1/\varkappa(r+1)]. \qquad (21)$$

The expression for the wave function $\alpha(n)$ differs from (21) in that $(r+1)$ is replaced by r.

Substitution of Eq. (20) in (18) and the use of (12) leads to the dispersion law

$$E(p)=E^{(0)}+E_p^{(1)},$$

where

$$E_p^{(1)}=-2\alpha^2(r+1)\Big|J(2r)+\sum_n\beta^2(n,n)J(r-n)$$

$$\times J(r+n)[E^{(0)}-K\beta^2(n,n)]^{-1}\Big|\cos 2p$$

$$=-(\pi^2a^2mA^2/8R^3\varkappa^3)\exp(-2\varkappa R)$$

$$\times\{1+(maA^2/4\varkappa)F(E^{(0)})\}\cos 2p,$$

$$F(E^{(0)})=\sum_{n=-r}^{r}\cos^2 qn[E^{(0)}(r+1)-\cos^2 qn]^{-1} \qquad (22)$$

and $E^{(0)}$ is determined from the integral equation

$$[E^{(0)}+2(r+1)J(0)]=-\alpha(r+1)\sum_n\beta^2(n,n)[J^2(r$$

$$+n)+J^2(r-n)]$$

$$\times[E^{(0)}-K\beta^2(n,n)]^{-1}. \qquad (23)$$

The first term in the expression for $E_p^{(1)}$ corresponds to the ferron motion due to the immediate exchange between f-spins at its boundaries, the second term to its magnon-assisted motion in the FM region.

Both lead to practically the same exponential dependence of the ferron band width on the ferron size (with an accuracy of a relatively weak R-dependence of F). As already pointed out in the preceding section at the direct f-f-exchange the ferron-band width exponentially decreases with increasing R, too, but according to (14) the exponent there is quite different.

MANY-ELECTRON FERRON

The distinguishing features of many-electron ferron motion are determined by two circumstances. Firstly, the indirect exchange influencing the positions of the ferron boundaries is carried out additively by all the N electrons of the ferron. This increases the mobility of a many-electron ferron compared to the one-electron ferron. But on the other hand, spin flip of one electron causes a reversal of one of the f-spins, i.e., a change in the f-spin configuration. The remaining $(N-1)$ s-electrons which preserved their spin projections should change their orbital states in order to become adjusted to the new configuration of f-spins. The necessity of reconstruction of these electron states hinders the f-spin flip, i.e., the ferron motion, and to larger degree the more electrons in the ferron. Formally, this manifests itself in a many-electron renormalization of the effective indirect-exchange integral.

In what follows we confine ourselves for simplicity only to indirect exchange directly connecting the ferron boundary atoms with each other. The basic wave functions are the following: the ground state wave function of the many-electron ferron

$$\psi_{2l}=\prod_{i=0}^{N-1}\alpha_{2l,i}\Phi_{2l}, \qquad (24)$$

and the wave functions describing virtual states with downward reversed spin of an electron initially in the jth state, and with upward reversed f-spin adjacent to the ferron boundary:

$$\psi_{2l+1,k,j}=\gamma_{2l+1,k}\prod_{i\neq j}\zeta_{2l+1,i}S_{2l+r+1}^+\Phi_{2l}. \qquad (25)$$

Here the electron wave functions $\alpha_{2l,i}$ and $\gamma_{2l+1,k}$ are the same as in (6), (7), and (15), and the wave functions

$$\zeta_{2l+1,i}=\sum\zeta_i(g-2l-1)a_{g,1/2}^*|0\rangle \qquad (26)$$

correspond to electron states in a ferromagnetic potential well of length $2(R+a)$, produced as a result of spin-reversal of one of atoms adjacent to the initial ferromagnetic potential well of length $2R$. The level number i corresponds here to the level numbering in the initial potential well. The product over i in (24) and (25) contains only the N lowest states, all occupied by electrons. The index j labels one of them.

Representing the wave function of the moving many-electron ferron as an expansion in the aforementioned eigenfunctions of the Hamiltonian H_0, i.e., in the form

$$\psi = \sum x_{2l}\psi_{2l} + \sum y_{2l+1,k,j}\tilde{\tilde{\psi}}_{2l+1,k,j}, \quad (27)$$

and acting on it by the Hamiltonian H (1), one obtains the following expression for the ferron spectrum:

$$E(p) = -(A^2/2)\sum_{j,k} \alpha_j^2 Q_j^2/E_{jk} - 2\sum_j J_j(2r)\cos 2p, \quad (28)$$

$$J_j(2r) = (A^2/4)\alpha_j^2(r+1)Q_j^2 \sum_k \gamma_k^*(2l-r+1)$$

$$\times \gamma_k(2l+r+1)/E_{kj}, \quad (29)$$

where the notation used is

$$Q_j = \prod_{i \neq j} (\zeta_{2l+1,i}, \alpha_{2l,i}). \quad (30)$$

As seen from comparing (28) and (29) with (17), the many-electron nature of the ferron has led, in addition to summation over all the occupied electron states, also to renormalization of the indirect-exchange integral J_j as manifested in its multiplication by the factor Q_j^2. When estimating this factor, if N is large, in the principal order in $1/r$, we can include in it also the omitted term with $i \neq j$. Using for α_i and ζ_i the wave functions of an electron in an infinitely deep potential well, we obtain

$$(\zeta_{2l+1,j}, \alpha_{2l,j}) = [r^{1/2}(r+1)^{1/2}/\pi j]\sin[\pi j/(r+1)]$$

$$\times [1 - \sin(\pi j)/(2r+1)]. \quad (31)$$

At $N \ll r$ one may write, using (30) and (31):

$$Q^2 = \prod_{j=0}^{N-1} \{1 - 1/(r+1) + 2\sin(\pi j)/(2r+1)$$

$$- (\pi^2/3r^2)(j+1)^2]$$

$$\approx \exp(-\pi^2 N^3/9r^2). \quad (32)$$

The character of dependence of the ferron bandwidth on the number of electrons in the ferron can be established as follows. Obviously, the quantity Q^2 (32) decreases monotonically with increase of N. But on the other hand, in the sum (28) there are N terms, i.e., approximately the one-electron indirect-exchange integral is multiplied by N. Hence, given R, the ferron energy-band width should be a nonmonotone function of N: first it should increase with N, and then, passing through the maximum at $N \approx (r^2/3)^{1/3}$, it should begin to decrease steeply. In other words, if the number of electrons in the ferron is not too large, its mobility is higher than that of a one-electron ferron. For a very large number of electrons its mobility is vanishingly small.

Strictly speaking, at fixed parameters of the crystal, but at variable conduction-electron density in it, the parameter R itself depends on the number of electrons in a ferromag-

netic droplet. But for real systems this dependence is not very strong[2] and for this reason does not influence the qualitative conclusion made above.

THE HOPPING MECHANISM OF FERRON MOTION

The expressions obtained above for the ferron band width evidence that the band mechanism of the ferron motion can be realized only in almost perfect crystals. In fact, if one assumes the following values of parameters typical of rare-earth compounds: $A \simeq 0.5$ eV, $W \simeq 3$ eV, $a \simeq 4$ Å (which corresponds to an electron effective mass of the order of the actual one), then according to (22) the ferron band width amounts only to 10^{-4}–10^{-5} eV at $R = 5a$ and 10^{-7} eV at $R = 10a$. Thus, potential fluctuations due to the imperfection of the crystal, should lead to the Anderson localization of the ferron at realistic imperfection degrees.

The band mechanism of the ferron motion should become inoperative also in not very weak external electric fields $\mathscr{E}$. In fact, at the ferron band widths indicated above they are so bent that the notion of the band spectrum loses its meaning: the band widths become less than the potential difference $2e\mathscr{E}a$ between two successive locations of the ferron center already at the field strengths 1-100 V/cm.

An alternative to the band mechanism is the hopping mechanism walks occurring with the energy exchange between the ferron and the magnons or phonons playing the part of the heat bath. The gap in the magnon spectrum [$\lambda > 1$ in (1)] hinder magnons in playing this part at low temperatures. It will be assumed in what follows that this part is played by acoustic phonons, and that the potential fluctuations are small enough so that ferron interstitial hops are accompanied by emission or absorption of only one acoustical phonon. The main regularities of ferron hops will be investigated below using the one-electron ferron as an example, neglecting magnetic disorder at $T \neq 0$.

First of all, the Hamiltonian (1) should be supplemented with a term

$$H_f = \sum_g E_g a_{g,\sigma}^* a_{g,\sigma} \quad (33)$$

that takes into account the electron energy differences between different sites (the energy E_g, assumed small compared with A, includes both the potential fluctuations and the external field). Further, the Hamiltonian H_{ph} of the acoustical phonons and the Hamiltonian H_3 of their interaction with the conduction electrons should be added to the Hamiltonian (1),

$$H_{ph} = \sum \omega_q b_q b_q, \quad (34)$$

$$H_3 = N^{-1/2}\sum G_q(b_q + b_{-q})a_{k,\sigma}^* a_{k+q,\sigma} \equiv H_3^{(+)} + H_3^{(-)}, \quad (35)$$

where b_q^* and b_q are the phonon operators, the electron-phonon coupling constant is assumed to be small, with $G_q \to 0$ at $q \to 0$, and N is the number of the unit cells in the crystal.

As in the preceding section, it will be assumed here that the ferron motion is the result of indirect exchange relating atoms at opposite boundaries of the ferron. We consider ferron transition from the state with the central atom 0 to the state with the central atom 2. This process proceeds as follows: 1) Owing to the Hamiltonian H_1 (1), the spins of the atom $(r+1)$ and of the s-electron reverse their direction, and the s-electron goes over into a free state. 2) In this state the electron emits or absorbs a phonon whose energy is equal to the difference of the electron energies in the considered ferron states with centers at the atoms 0 and 2. Such a one-phonon scattering act is caused by the Hamiltonian H_3 (35). 3) Owing to the Hamiltonian H_1 spin reversals of the atom $(-r+1)$ and the s-electron occur, with transition of the latter into the ferromagnetic region centered at the atom 2.

Thus, to calculate the probability P_{02} of the ferron transition from the atom 0 to the atom 2, one should use the sixth order of the time-dependent perturbation theory in the Hamiltonian H_1+H_3. The corresponding expression is deduced in standard fashion and in a quadratic approximation for the electron spectrum it can be presented in the form

$$P_{02}=2\pi \sum_q \langle|M_q^{(\pm)}|^2\rangle\delta(\bar{E}_2-\bar{E}_1 \mp \omega_q), \qquad (36)$$

$$\bar{E}_{2l}= \sum_g E_g \alpha^2(g-2l), \qquad (37)$$

$$M_q^{(\pm)}= \sum_k (\psi_0,H_1\tilde{\psi}_{1,k})(\Omega_{n_q}\gamma_k,H_3^{(\pm)}\gamma_{k\pm q}\Omega_{n_q\pm1})$$

$$\times(\tilde{\psi}_{1,k\mp q},H_1\psi_2)(A/4+k^2/2m)^{-1}$$

$$\times[A/4+(k\mp q)^2/2m]^{-1}, \qquad (38)$$

where ψ_{2l} and $\tilde{\psi}_{2l+1,k}$ are given by Eqs. (7) and (15), Ω_{n_q} is the wave function of phonons with momentum q corresponding to their number n_q. The angular brackets denote thermodynamic averaging over the phonons. In the energy denominator of (38) the term ω_q is discarded because of its small value.

With allowance for the structure of the Hamiltonian H_3 (35), the calculation of $M_q^{(\pm)}$ reduces virtually to integration in the expression

$$\int_{-\infty}^{\infty} dk \exp\{-2kri\pm i(-r+1)q\}(\varkappa^2+k^2)^{-1}$$

$$\times[\varkappa^2+(k\pm q)^2]^{-1},$$

which is easily achieved by residue theory. The result is

$$P_{02}=(2\pi A^4 m^4 a^2/N\varkappa^2)\exp(-4\varkappa R)\sum G_q^2 q^{-2}$$

$$\times[q\cos qr+2\varkappa\sin qr]^2[v_q\delta(e\bar{E}_2-\bar{E}_0-\omega_q)$$

$$+(v_q+1)\delta(\bar{E}_2-\bar{E}_0+\omega_q)][q^2+4\varkappa^2]^{-2}, \qquad (39)$$

where v_q is the average number of phonons with momentum q.

As follows from (39), the transition probability also exhibits an exponential dependence on the ferron size which is even more sharp than the ferron band width. In a similar manner, P_{02} increases with A/W, and so does the ferron band width. The probability P_{02} for a many-electron ferron at not very large numbers N of electrons in it increases with N as N^2 (see the preceding section). Thus, the kinetic characteristics obtained by an analysis of the ferron band agree qualitatively with those obtained from the expression for the transition probability.

APPENDIX
FERRONS IN MAGNETIC SYSTEMS WITH ARBITRARY ATOM SPINS

The calculation presented above is restricted to magnets with spins equal to 1/2. One may expect that at larger spins the system should behave like a classical one, i.e., that the ferron bandwidth should tend to zero. To prove this statement, a calculation is carried out below for the case when the ferron motion is caused by a direct displacement of the ferron boundaries. But a change in the orientation of spins $2l+(r-1)$ inside the ferron and $2l-(r+1)$ outside it as it moves to the left (and of corresponding pair of spins as the ferron moves to the right) occurs via a series of successive spin rotation with change in their projections by ±1, until their total change reaches $\pm2S$.

Since the total spin projection of the system should remain unchanged, in the first approximation in A/W the energy of the s-electron does not change, this is equivalent to the use of a model magnetic Hamiltonian of the type

$$H=-I\sum\{S_{2l+r+1}^+ S_{2l-r+1}^- + S_{2l-r+1}^- S_{2l-r+1}^+$$

$$+S_{2l-r-1}^+ S_{2l+r-1}^- + S_{2l-r-1}^- S_{2l+r-1}^+\} \qquad (40)$$

(the r-dependence of the effective exchange integral I is not discussed here).

The wave function of the ferron is constructed as follows:

$$\Phi=\sum_l \left\{x_{2l}+\sum_{n=1}^{2S-1} C_n[y_{2l,n,2l+2}(S_{2l-r+1}^-)^n(S_{2l+r+1}^+)^n\right.$$

$$\left.+y_{2l,n,2l-2}(S_{2l-r+1}^-)^n(S_{2l-r-1}^+)^n]\right\}\Phi_{2l}, \qquad (41)$$

where Φ_{2l} is given by Eq. (5) and C_n is the normalization factor.

The coefficients of the expansion (40) are found from equations obtained with the aid of (40):

$$\varepsilon x_{2l}=T_0(y_{2l,1,2l-2}+y_{2l,1,2l+2}),$$

$$\varepsilon y_{2l,n,2l-2}=T_n y_{2l,n+1,2l-2}+T_{n-1}y_{2l,n-1,2l-2}$$

$$\times(2S-1>n>1),$$

$$\varepsilon y_{2l,1,2l-2}=T_0 x_{2l}+T_1 y_{2l,2,2l-2},$$

$$\varepsilon y_{2l,2S-1,2l-2}=T_0 x_{2l-2}+T_1 y_{2l,2S-2,2l-2}, \qquad (42)$$

and similar equations for $y_{2l,n,2l+2}$. The notations used here are

$$T_n = (n+1)(2S-n), \quad \varepsilon = E/J.$$

At relatively small S one can obtain a solution of the set of equation (42) in explicit form:

$$q = \cos^{-1} \varepsilon/4, \quad (S=1)$$

$$q = \cos^{-1}\{\varepsilon(\varepsilon^2 - 2)/24\}, \quad (S=3/2) \text{ and so on,}$$

(43)

where q is the ferron quasimomentum.

But at large S one can only obtain a lower-limit estimate for the moving ferron energy and an upper-limit estimate for the ferron bandwidth W_F. To this end it is sufficient to set in (43) all the values of T_n except T_0 equal to the maximum value $T_m = S^2 - 1/4$. Then the upper limit for the bandwidth is given by the relation

$$W_F/|J|S^2 < \pi^2/2(S-2)^2 \ll 1$$

(44)

(W_F should be compared with the magnetic ordering energy $\tilde{I}S^2$ and not with the exchange integral $\tilde{I}$). According to estimates (43,44) the ferron bandwidth becomes negligibly small compared to the exchange-interaction energy only at nonphysically large spin values exceeding, at least, 5. This confirms the possibility of observing ferron motion in europium chalcogenides with $S=7/2$, as discussed in the Introduction.

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