Density of states tails in semimagnetic semiconductors

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A first theoretical look is taken at the tails of the density of states in semimagnetic semiconductors. The exchange interaction between a charge carrier and magnetic ions makes the energy dependence of the density of states $g(E)$ in the tails markedly different from the known energy dependence $g_0(E) \propto \exp[-(|E|/\varepsilon_0)^{1/2}]$ for nonmagnetic solid solutions. The $g(E)$ dependence is not monotonic. Some characteristic energies $E_1 < E_f < E_2 < 0$ which separate spectral regions with qualitatively different $g(E)$ behavior are found. There is a $g_0(E)$ dependence only at the lowest energies, $|E| \ll |E_2|$. At $E_f < E < E_2$ the density of states again falls off with increasing $|E|$, but it is exponentially larger than $g_0(E)$. In the region $E_1 < E < E_f$ the density of states has a deep valley. Finally, at the lowest energies $E < E_1$ there is a dependence $g(E) \propto \exp[-(|E|/\varepsilon_1)^{1/2}]$, where ε_1 may be several times ε_0. The thermal disorder in the spin system of the ions makes the density of states $g(E)$ temperature-dependent. Some possible experimental manifestations of these features of the tails on the density of states are discussed.

1. INTRODUCTION

Fluctuations in the chemical composition of solid solutions are known to give rise to tails on the density of states (Refs. 1–3, for example). If there is no spatial correlation in the arrangement of the atoms of the solution, the energy dependence of the density of states is described by

$$g(E)=g_0\exp[-\Phi_0(E)],\quad \Phi_0(E)=(|E|/\varepsilon_0)^{1/2}. \tag{1}$$

The tail decay parameter is determined by the nature and extent of the disorder. For a substitutional disorder, for example, we would have

$$\varepsilon_0=\frac{(va^{-3})^4}{cB^3}(\bar{n}a^3)^2,\quad B\equiv\frac{\hbar^2}{ma^2}, \tag{2}$$

where v is the effective potential of one impurity atom, $\bar{n}$ is the average impurity concentration, a is a lattice constant, m is the effective mass of the charge carrier, and $c \approx 178$ is a numerical factor.[2–4] The results in (1) and (2) describe the tails on the density of states in nonmagnetic semiconductors, where the interaction of an electron with impurity atoms is caused exclusively by the properties of the core potentials of the atoms.

In this paper we will be discussing semimagnetic semiconductors, which are usually thought of as solid solutions in which one component has a net magnetic moment. Examples are the solid solutions $M_xA^{\rm II}_{1-x}B^{\rm VI}$, in which the magnetic impurity M is an iron-group atom. The exchange interaction with the atoms of the magnetic impurity strongly influences the properties of the charge carriers in semimagnetic semiconductors.[5] In particular, it should affect the shape of the tails on the density of states. This topic, which has not been discussed previously, is the subject of the present paper.

We consider a solid solution with a relatively low concentration of the magnetic impurity, $\bar{n}a^3 \ll 1$, at temperatures T which are not too low, at which there is no magnetic order. The interaction of an electron with the impurity system is described by the Hamiltonian

$$H=-J\sum_i\delta(\mathbf{r}-\mathbf{r}_i)(\mathbf{s}\mathbf{S}_i)+v\sum_i\delta(\mathbf{r}-\mathbf{r}_i), \tag{3}$$

where J is the exchange-interaction integral. The summation in (3) is over all the impurity centers, $\mathbf{S}_i$ is the spin of impurity center i, and $\mathbf{s}$ is the spin of an electron ($s = 1/2$). To help clarify the discussion below, we will cite some typical values of the parameters in (3). For the materials which have been studied in most detail, $\mathrm{Cd}_{1-x}\mathrm{Mn}_x\mathrm{Te}$ and $\mathrm{Hg}_{1-x}\mathrm{Mn}_x\mathrm{Te}$, the quantity $|Ja^{-3}|$ is ~ 1 eV, slightly different for electrons and holes. The quantity v, which stems from the difference between the core potentials of the impurity and host atoms, should be on the order of atomic scales, i.e., $|va^{-3}| \gtrsim 1$ eV. The parameter va^{-3} can also be estimated from the concentration dependence of the width of the band gap, G:

$$va^{-3}=dG/dx.$$

From the data of Ref. 5, we find that va^{-3} varies with the particular material, from 0.5 eV ($\mathrm{Zn}_{1-x}\mathrm{Mn}_x\mathrm{Te}$) to ~ 4 eV ($\mathrm{Hg}_{1-x}\mathrm{Mn}_x\mathrm{Te}$). The value of $S = |\mathbf{S}|$ is usually a few units; for Mn^{2+} ions, for example, it is $S = \frac{5}{2}$. The situation $|v| \sim |JSs|$ is thus typical, and this is the situation on which we focus below. When we take up the relatively improbable although theoretically possible case $|v| \ll |JSs|$, we will state so explicitly. We would point out, however, that for the exchange interaction to outweigh the potential interaction we would actually need the stiffer condition $|v| \ll |J\bar{S}s|$, where $\bar{S}$ is the average spin induced by the field of an electron, which satisfies $|\bar{S}| \leqslant S$.

The discussion below is organized as follows. In Sec. 2 we present some qualitative arguments which will make it possible to describe, without further calculations, the energy dependence of the density of states in a semimagnetic semiconductor. In Sec. 3 we use an optimum-fluctuation method to derive explicit expressions for $g(E)$ in semimagnetic semiconductors in various energy regions. Section 4 contains a discussion of the results.

2. QUALITATIVE CONSIDERATIONS

We begin with a description of the effect of the exchange interaction on the properties of localized electrons in a semimagnetic semiconductor. The most important consequence of this interaction for our purposes is the magnetopolaron effect.[6] This effect can be summarized by saying that a localized electron orients the spins of the magnetic atoms, so a self-consistent magnetization arises. It lowers the energy of the system. In describing such states, it is convenient to distinguish three regimes, which correspond to different temperatures.

Saturation regime. This regime is realized at the lowest temperatures, at which essentially all the spins in the electron localization region are oriented. This case occurs under the condition

$$|JSs|\langle|\psi(\mathbf{r})|^2\rangle/T\gg 1. \tag{4}$$

Here $\psi(\mathbf{r})$ is the electron wave function, and the angle brackets mean an average over the localization region.

Polaron regime. This regime arises with increasing T, when inequality (4) is reversed. In this regime the response of the magnetic impurity system to the electron spin becomes linear in the parameter $|JSs|\langle\psi^2\rangle/T\ll 1$. The effective field acting on an electron turns out to be proportional to $\psi^2\equiv|\psi(\mathbf{r})|^2$, as in the case of ordinary acoustic polarons.[7] The corresponding states are magnetic polarons in a random field generated by fluctuations in the concentration of the magnetic impurity. In this regime, thermal fluctuations of the spins of the magnetic atoms are substantial. However, their nonvanishing average magnetization is still important.

Thermodynamic-fluctuation regime. This regime occurs at the highest temperatures. Here the fluctuations of the magnetization of the atomic spin system exceed the average value of the magnetization. The electron is coupled with the fluctuating magnetization because the electron spin and the spatial variations of the magnetization make local "fine adjustments" of the approximate nature. The temperature at which this regime begins to set in can be estimated by equating the energy of the interaction of an electron with N atoms in the localization region, i.e., $|JSs|\psi^2N$, to the energy of the thermal fluctuations, i.e., $N^{1/2}T$. Here one must bear in mind that $N\sim\bar{n}R^3$, where R is the localization radius. The normalization condition $\psi^2R^3\approx 1$ must also be taken into account. As a result, the condition for the thermodynamic-fluctuation regime becomes

$$\bar{n}J^2(Ss)^2\langle\psi^2\rangle/T^2\ll 1. \tag{5}$$

Since $N\gg 1$ and $|J\bar{n}/T|\gg 1$, the temperature of the transition to the regime of thermodynamic fluctuations is much higher than the temperature of the transition from the saturation regime to the polaron regime. There is accordingly a region in which the polaron regime exists.

We will now use the discussion above to describe the behavior of the density of states in the tails in a semimagnetic semiconductor. We note first that conditions (4) and (5) can be used to distinguish different energy regions in the tail on the density of states at a fixed temperature. The idea is that as the state energy E in the band gap decreases there is a decrease in its localization radius, and $\langle\psi^2\rangle\sim R^{-3}$ correspondingly increases. It follows that at a given temperature T there is a characteristic energy $E_1(T)$ which separates the regions of the saturation and polaron regimes:

$$\begin{aligned} &|JSs|\langle\psi^2\rangle/T>1, \quad E<E_1(T),\\ &|JSs|\langle\psi^2\rangle/T<1, \quad E>E_1(T). \end{aligned} \tag{6}$$

Correspondingly, one can introduce an energy $E_2(T)$ which separates the regions of the polaron and thermodynamic fluctuation regimes:

$$\begin{aligned} &\bar{n}J^2(Ss)^2\langle\psi^2\rangle/T^2>1, \quad E<E_2(T),\\ &\bar{n}J^2(Ss)^2\langle\psi^2\rangle/T^2<1, \quad E>E_2(T). \end{aligned} \tag{7}$$

In the saturation regime, i.e., at $E<E_1$, essentially all the spins of the magnetic atoms are oriented, so the energy of the interaction with each of them changes by the maximum possible amount:

$$v\to v-{}^1/_2|JS|. \tag{8}$$

In addition, the origin of the energy scale shifts by an amount $|JS|\bar{n}/2$. As a result, the tail on the density of states at $E<E_1$ can be described by expressions (1) and (2), in which it is sufficient to make the substitution

$$E\to E+{}^1/_2|JS|\bar{n}, \quad \varepsilon_0\to\varepsilon_1=\varepsilon_0[(v-{}^1/_2|JS|)/v]^4. \tag{9}$$

The exchange interaction in a semimagnetic semiconductor thus leads to an exponential variation of the tails on the density of states at $E<E_1(T)$.

We turn now to an analysis of the polaron energy region, $E_1(T)<E<E_2(T)$. In this region, the localization radius of the state increases with increasing $E(>E_1)$, and the coupling of the electron with the magnetic moments of the atoms weakens. One might expect that the destruction of magnetic polarons by the thermal disorder in this energy region would lead to a valley in the density of states. We should thus find a peak in the density of states at $E\sim E_1$.

In the region of the thermodynamic-fluctuation regime, $0<E<E_2(T)$, the magnetic interaction of the electron with the impurity ions leads to a relatively slight lowering of the electron energy, $|\Delta E|\ll|E|$. Correspondingly, the shape of the tails on the density of states should be approximately as described by (1):

$$\Phi_0(E)=\left(\frac{|E|}{\varepsilon_0}\right)^{1/2}\left(1-\alpha\left|\frac{\Delta E}{E}\right|\right), \tag{10}$$

where α is a numerical coefficient. To estimate ΔE we note that at high temperatures the interaction with the magnetic ion induces an average spin $\bar{s}\sim JS\psi^2/T$ at an electron. As a result we find

$$\Delta E\sim|JS\bar{s}|n\sim J^2S^2\psi^2n/T. \tag{11}$$

In the region of thermodynamic fluctuations of the density of states, $g(E)$ therefore increases with increasing E. To conclude this section of the paper we note that localization effects in the tails on the density of states can be important only at fairly low temperatures. Specifically, the thermal energy T must be considerably lower than the maximum energy scale in the tail on the density of states. We therefore assume

$$T\ll\max\{\varepsilon_0,\ \varepsilon_1,\ |JS|\bar{n}/2\}.$$

3. OPTIMUM-FLUCTUATION METHOD

Our problem is to find the explicit expression for the function $\Phi_0(E)$ at high energies $|E|$ in the region of an exponentially low density of states:

$$g(E)=g_0\exp[-\Phi_0(E)]\ll g_0.$$

In this region, among all possible local configurations of the impurity center which would create electronic states with a given energy E, there are certain optimum configurations which dominate $g(E)$. The optimum-fluctuation method[1,2] makes it possible to determine such configurations and their contribution to $\Phi_0(E)$. A specific feature of out problem is that we are dealing with states with a given free energy F. This formulation of the problem is dictated by the need to deal with thermodynamic fluctuations in a spin system. We thus seek the optimum fluctuations which determine the density of states for a given value of F. In this case the density of states can be thought of as a function of the free energy F or as a function of the electron energy E corresponding to the given value of F.

We consider the Gaussian region of the spectrum, where the density of states remains appreciable in magnitude. In this region, the situation is dominated by fluctuations created by a relatively small deviation of the local impurity concentration $n(\mathbf{r})$ from its average value $\bar{n}$. The probability for the formation of a fluctuation $\delta n(\mathbf{r})$ is

$$\exp\left[-\int d\mathbf{r}\frac{\delta n^2(\mathbf{r})}{2\bar{n}}\right], \tag{12}$$

where $\delta n(\mathbf{r}) = n(\mathbf{r}) - \bar{n}$. Optimizing probability (12) for a given value of F is equivalent to seeking an extremum of the functional

$$\Phi[n(\mathbf{r})]=\int d\mathbf{r}\frac{\delta n^2(\mathbf{r})}{2\bar{n}}-\lambda\left[F-\mathscr{E}\int\psi^2(\mathbf{r})\,d\mathbf{r}\right], \tag{13}$$

where λ and $\mathscr{E}$ are Lagrange multipliers. The last term in (square) brackets in (13) reflects the fact that the electron wave function in a fluctuation is normalized. We will see below [see (22)] that $\mathscr{E}$ is the self-energy of an electron.

The free energy F is given by

$$F=\frac{\hbar^2}{2m}\int(\nabla\psi(\mathbf{r}))^2\,d\mathbf{r}+v\int\psi^2(\mathbf{r})\,n(\mathbf{r})\,d\mathbf{r}-T\ln Z, \tag{14}$$

where Z is the partition function of the spin system, given by

$$Z=\operatorname*{Sp}_{\mathbf{s}}\operatorname*{Sp}_{\mathbf{S}_i}\exp\left[J\sum_i\frac{(\mathbf{S}_i\mathbf{s})\psi^2(\mathbf{r}_i)}{T}\right]. \tag{15}$$

Using standard manipulations,[8] we can put Z in the form

$$Z=2\prod_i f(\xi_i)\left[1+\sum_i\xi_i B_S(\xi_i)\right]. \tag{16}$$

Here

$$\xi_i=\frac{J}{2T}\psi^2(\mathbf{r}_i), \tag{17}$$

$$f(\xi)=\frac{\operatorname{sh}[(S+{}^1/_2)\xi]}{\operatorname{sh}(\xi/2)}, \tag{18}$$

$$B_S(\xi)\equiv\frac{f'(\xi)}{f(\xi)}=\left(S+\frac{1}{2}\right)\operatorname{cth}\left[\left(S+\frac{1}{2}\right)\xi\right]-\frac{1}{2}\operatorname{cth}\frac{\xi}{2}. \tag{19}$$

The function $B_S(\xi)$ is the ordinary Brillouin function.

Using (14) and (16)–(19), we can vary functional (13) with respect to $\psi(\mathbf{r})$ and $\delta n(\mathbf{r})$. Switching from a summation over the sites i to an integration, and equating the variation $\delta\Phi$ to zero, we obtain the system of equations

$$\begin{gathered}-\frac{\hbar^2}{2m}\Delta\psi-\left[\frac{1}{2}JnB_s(\xi)-vn\right]\psi-\frac{1}{2}Jn\frac{\xi B_S'(\xi)+B_S(\xi)}{1+I}\\=\mathscr{E}\psi,\\\delta n+\lambda\bar{n}[v\psi^2-T\ln f(\xi)]-\lambda T\bar{n}\xi B_S(\xi)/(1+I)=0.\end{gathered} \tag{20}$$

Here we have introduced

$$I=\bar{n}\int\xi(\mathbf{r})B_S[\xi(\mathbf{r})]\,d\mathbf{r}. \tag{21}$$

Equations (20) lead to an equation of the Schrödinger type with a ψ-dependent effective potential:

$$-\frac{\hbar^2}{2m}\Delta\psi+U\psi=E\psi,\quad E=\mathscr{E}-v\bar{n}. \tag{22}$$

The energy E is reckoned from the shifted band boundary, as in (1):

$$\begin{aligned}U=&\left\{v\bar{n}-\frac{1}{2}J\bar{n}B_S(\xi)\left[1+\frac{1+\xi B_S'(\xi)/B_S(\xi)}{1+I}\right]\right\}\\&\cdot\Big\{1-\lambda\Big[v\psi^2-T\ln f(\xi)-\frac{1}{2}J\frac{B_S(\xi)}{1+I}\psi^2\Big\}-v\bar{n}.\end{aligned} \tag{23}$$

In addition, using Eqs. (20), we can express the argument of the exponential function in the density of states in terms of λ and ψ:

$$\Phi_0(E)=\min_{\delta n(\mathbf{r})}\int d\mathbf{r}\frac{\delta n^2(\mathbf{r})}{2\bar{n}}.$$

We then find

$$\Phi_0(E)=\frac{\bar{n}}{2}\lambda^2\int d\mathbf{r}\left[v\psi^2-T\ln f(\xi)-\frac{{}^1/_2JB_S(\xi)}{1+I}\psi^2\right]^2. \tag{24}$$

To determine an explicit expression for the functional dependence $\Phi_0(E)$ we should work from the solution of Eq. (22) to find the function $\psi(\mathbf{r})$ and $\lambda(E)$ and then substitute them into (24). This procedure cannot be implemented analytically for arbitrary values of the parameters in (22)–(24). We will thus consider separately the various parts of the spectrum according to the classification given in Sec. 2.

As follows from (4), the saturation regime corresponds to the condition $\xi\gg1$. In this case the following approximations hold:

$$B_S(\xi)\approx S\operatorname{sign}J,\quad\ln f(\xi)\approx\frac{|JS|}{2T}\psi^2,\quad I\approx\frac{|JS|\bar{n}}{2T}\gg1. \tag{25}$$

Equation (22) becomes

$$-\frac{\hbar^2}{2m}\Delta\psi-\lambda\bar{n}\left(v-\frac{|JS|}{2}\right)^2\psi^3=\left(E+\frac{|JS|\bar{n}}{2}\right)\psi. \tag{26}$$

A nonlinear Schrödinger equation of the type in (26) has been studied in detail in papers on the standard optimum-fluctuation method.[1-3,9] The results of importance here can be summarized by the expressions

$$\begin{gathered}E+\frac{|JS|}{2}\bar{n}=-\frac{c}{4}\frac{\hbar^6}{m^3}\left[\bar{n}\lambda\left(v-\frac{|JS|}{2}\right)^2\right]^{-2},\\\int\psi^4\,d\mathbf{r}=c\frac{\hbar^6}{m^3}\left[\bar{n}\lambda\left(v-\frac{|JS|}{2}\right)^2\right]^{-3}.\end{gathered} \tag{27}$$

Using these results, we obtain expressions (1) and (2) with the parameters in (9). Where necessary we can also express the density of states in terms of the free energy, which in the case at hand is

$$F=E-T\ln2\left(1+\frac{|JS|\bar{n}}{2T}\right). \tag{28}$$

We turn now to the polaron regime, in which we again have $I\gg1$ but $\xi\ll1$. We can use the following approximations in this case:

$$B_s \approx \frac{S(S+1)}{6T}\psi^2, \quad \ln f(\xi) \approx \frac{S(S+1)}{6}\left(\frac{J}{2T}\psi^2\right)^2,$$
$$I \approx \frac{S(S+1)}{3}\left(\frac{J}{2T}\right)^2 \bar{n} \int \psi^4\, d\mathbf{r}. \tag{29}$$

Equation (22) becomes

$$-\frac{\hbar^2}{2m}\Delta\psi - \bar{n}\left[\lambda v^2 + \frac{S(S+1)}{12T}J^2\right]\psi^3 = E\psi. \tag{30}$$

There is a difference between Eqs. (30) and (26) in that λ appears in only one of the two terms in the effective potential. However, expressions of the type in (27), suitably modified, are again applicable. Using them, we find

$$\Phi_0(E) = \left(\frac{|E|}{\varepsilon_0}\right)^{1/2}\left[1 - \left(\frac{|E|}{\varepsilon^*}\right)^{1/2}\right]^2,$$
$$\varepsilon^* = \frac{T^2}{\varepsilon_0}\left[\frac{6v^2}{S(S+1)J^2}\right]^2. \tag{31}$$

The free energy is expressed in terms of E:

$$F = E\left[1 - 2\left(\frac{|E|}{\varepsilon^*}\right)^{1/2}\right] - T\ln\left[\frac{8\varepsilon^*}{T}\left(\frac{|E|}{\varepsilon^*}\right)^{3/2}\right]. \tag{32}$$

For the values under consideration, $|E| \gg T$, the free energy has a minimum as a function of the energy E at

$$|E_f| \approx \frac{\varepsilon^*}{9}\left(1 + \frac{27}{2}\frac{T}{\varepsilon^*}\right). \tag{33}$$

The existence of this minimum means that there are no states with energies $E < E_f$ in the polaron regime. The valley in the spectrum of the density of states in the case with a polaron effect was first observed by Kusmartsev and Rashba.[9]

Our last topic is the thermodynamic-fluctuation regime. In this case approximations (29) remain valid, but we have $I \ll 1$. Equation (22) accordingly takes the form (30) with the second term of the effective potential greater by a factor of 3. It thus becomes possible to formally make use of expressions (31) with $\varepsilon^* \to \varepsilon^*/9$. In this regime the second term in (31) is small, so we have

$$\Phi_0(E) \approx \left(\frac{|E|}{\varepsilon_0}\right)^{1/2}\left[1 - 6\left(\frac{|E|}{\varepsilon^*}\right)^{1/2}\right]. \tag{34}$$

Correspondingly, the free energy becomes

$$F = E[1 - 10(|E|/\varepsilon^*)^{1/2}] - T\ln 2. \tag{35}$$

To verify that $(|E|/\varepsilon^*)^{1/2} \ll 1$ is small, we need to express this quantity in terms of the parameter $I \ll 1$. Using expressions (27) for this purpose, we find

$$\left(\frac{|E|}{\varepsilon^*}\right)^{1/2} = \frac{T}{|E|} I \ll 1. \tag{36}$$

Expression (34) agrees with the qualitative result in (10) if we use the estimate $\psi^2 \sim R^{-3} \sim a^{-3}|E/B|^{3/2}$ in the latter.

We can now write expressions for the characteristic energies E_1 and E_2, which separate the regions in which these three regimes occur. These energies are determined from the conditions $\xi = 1$ and $I = 1$. In writing the first condition we express ψ^2 in terms of I. For this purpose we note that the potential well corresponding to the optimum fluctuation is approximately square,[1,2] and we adopt the approximation

$$\psi^2 = \int \psi^4\, d\mathbf{r}.$$

For I we use (36). As a result we find

$$|E_1| = [\varepsilon^*(\bar{n}J)^2]^{1/3}\left[\frac{S(S+1)}{24}\right]^{2/3} + \frac{|JS|\bar{n}}{2}, \quad |E_2| = (\varepsilon^* T^2)^{1/3}. \tag{37}$$

The second term in the expression for E_1 incorporates the shift of the origin for the energy scale [see (9)]. The relation $|E_1| \gg |E_2|$ between these energies is determined by the inequality $1/2|JS|\bar{n} \gg T$. The latter expresses the condition that the thermal energy is small in comparison with the maximum energy of the coupling of the electron with the magnetic moments of the impurity ions. Only in this case can the effects of the magnetic interaction be seen against the background of the thermal disorder.

The same inequality, $1/2|JS|\bar{n} \gg T$, guarantees satisfaction of the condition $E_f > E_1$. It means that there exists a gap in the density of states at $E_1 < E < E_f$ (Fig. 1). It should be kept in mind, however, that the conclusion that there is a gap applies only to the case of the Gaussian fluctuations under consideration here. When we take non-Gaussian fluctuations into account, we can say no more than that there exists an exponentially deep valley in the density of states between E_f and E_1. The most important feature of the picture which has been drawn is a peak in the density of states at energies $E \sim E_1$. An estimate of the density of states g_b at the peak yields

$$g_b \sim g_0 \exp\left[-\left(\frac{|E_1| - {}^1/_2|JS|\bar{n}}{\varepsilon_1}\right)^{1/2}\right].$$

When we substitute (37) in, we find

$$g_b \sim g_0 \exp\left[-\left(\frac{T}{T^*}\right)^{2/3}\right], \quad T^* = \frac{4\varepsilon_0^2 J}{v^2\bar{n}}\left(\frac{v - {}^1/_2|JS|}{v}\right)^6. \tag{38}$$

We conclude this section with a brief look at the hypothetical case $|v| \ll |J\bar{S}s|$. In this case the terms in the original Schrödinger equation, (22), which are small in proportion to the parameter

$$\left|\frac{v}{J\bar{S}s}\right| \sim \left|\frac{J^2S(S+1)}{12Tv}\psi^2\right|^{-1} \ll 1$$

are discarded. It is easy to see that in the saturation regime there is nothing in this case which is different from that in the

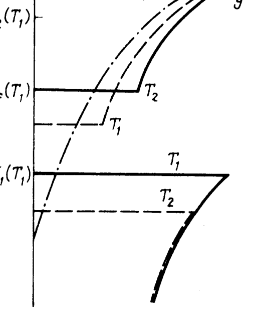

FIG. 1. Density of states in the tail in a semimagnetic semiconductor at temperatures T_1 and T_2. The dot-dashed line shows the density of states in the absence of an exchange interaction ($T_1 < T_2$).

case which we have already discussed: The density of states is described by Eqs. (1) and (2) with the renormalized parameters from (9).

For the polaron regime, the form of Eq. (22) now depends on the parameter $IT/|E|$. When it is small we have

$$-\frac{\hbar^2}{2m}\Delta\psi-\frac{1}{2}\bar{n}\lambda\left[\frac{J^2S(S+1)}{12T}\right]^2\psi^7=E\psi. \tag{39}$$

An approximate solution, within a numerical factor, yields an argument of the exponential function in the density of states which falls off with the energy:

$$\Phi_0(E)=\left(\frac{\varepsilon_v}{|E|}\right)^{5/2},\qquad \varepsilon_v\approx B\left[\frac{BTa^6}{J^2S(S+1)(\bar{n}a^3)^{1/2}}\right]^{4/5}. \tag{40}$$

At large values of the parameter, $IT/|E|\gg 1$, Eq. (22) becomes the Schrödinger equation for a free magnetic polaron:

$$-\frac{\hbar^2}{2m}\Delta\psi-\frac{J^2S(S+1)\bar{n}}{12T}\psi^3=E\psi. \tag{41}$$

This equation has no parameters which are associated with fluctuations of the concentration $n(\mathbf{r})$. This equation yields a peak in the density of states at the energy of a free polaron [see (27)]:

$$|E_p|=\frac{36cB^3T^2}{(Ja^{-3})^4[S(S+1)\bar{n}a^3]^2}. \tag{42}$$

The condition $J^2(S+1)S\bar{n}/12T>B$, which is the condition for the existence of a polaron state, along with the condition $IT/|E|>1$, which is the condition for the validity of Eq. (41), is summarized by the inequality

$$|E_p|>\frac{S(S+1)}{12}|J|\bar{n}. \tag{43}$$

In the thermodynamic fluctuation regime we have a parameter $IT/|E|\ll 1$. In this case Eq. (22) reduces to the form in (38), with an effective potential increased by a factor of 9. The result for $\Phi_0(E)$ is given by (40), in which ε_v must be replaced by $\varepsilon_v/3^{4/5}$.

We thus see that in the hypothetical case of small values of the impurity potential, $|v|\ll|J\bar{S}s|$, the density of states has a peak (Fig. 2). This peak occurs either at $E\sim E_p$ or near $E\sim E_1$, depending on whether inequality (43) does or does not hold.

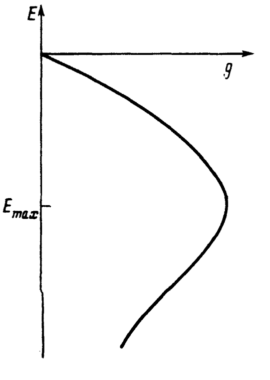

FIG. 2. Tail on the density of states in a semimagnetic semiconductor under the condition $|v|\ll|J\bar{S}s|$. Here $E_{\max}=E_p$ for the case $|E_p|>S(S+1)|J|\bar{n}/12$ and $E_{\max}=E_1$ for $|E_p|<S(S+1)|J|\bar{n}/12$.

4. DISCUSSION OF RESULTS; CONCLUSION

The basic result of this study is the prediction of a nonmonotonic energy dependence of the tails on the density of states in semimagnetic semiconductors. The observed deviation from a monotonic behavior is described by several energy parameters, which we will now estimate. For definiteness we assume the typical values $-va^{-3}\sim 3/4|JSa^{-3}|\sim 1.5$ eV, $\varepsilon_0\sim$ 1–10 meV, and $\bar{n}a^3\sim 0.1$ From expressions (9), (37), (33), and (38) we then find

$$\varepsilon_1\approx 8\varepsilon_0,\quad |E_1|\sim\frac{|JS|\bar{n}}{2}\sim 0{,}1\ \text{eV},\quad |E_2|\approx\varepsilon_0\left(\frac{T}{\varepsilon_0}\right)^{4/3},$$
$$|E_f|\approx\frac{\varepsilon_0}{4}\left(\frac{T}{\varepsilon_0}\right)^2,\quad T^*\sim 3-300\ \text{K}. \tag{44}$$

If $v>0$, then we obviously have $\varepsilon_1<\varepsilon_0$. We will not consider the unlikely case of the exact equality $v=|JS|/2$, in which we would have $\varepsilon_1=0$. Figure 1 shows the relative positions of the characteristic energies in the spectrum. Estimates (44) show that there exists a wide temperature range $\varepsilon_0\ll T\ll|E_1|$ in which the structure of the spectrum in Fig. 1—i.e., $|E_1|\gg T, |E_f|\gg T, |E_2|\gg T$—might be observable.

Let us explain the evolution of the spectrum with increasing temperature shown in Fig. 1. At extremely low values of T the localization of a charge carrier in the tail is accompanied by a complete polarization of the spins in the corresponding region and by a downward energy shift of the state to $E<E_1$. Consequently, at $T<\varepsilon_0$, there are essentially no states with energies $E_f<E<0$. With increasing T, the spin polarization effects weaken. Accordingly, there is no downward shift of the states with $E>E_f$ which are localized comparatively weakly, while the more localized states with $E<E_f$ undergo a shift as before. At the same time, the weakening of the polarization effects with increasing T leads to a destruction of the least bound states near the peak. The energy E_1 thus shifts downward. In the limit of very high values of T, the density of states corresponds to the ordinary law, (1).

It should be stressed that the nonmonotonic behavior of the tails on the density of states stems from the interaction of localized charged carriers with the spins of magnetic ions. For this reason, the nonmonotonic behavior of the tails could be seen only in processes involving initially localized carriers. Luminescence might be one such process. According to our results, the emission should be dominated by carriers which are localized in the peaks in the density of states at $E\sim E_1$. This conclusion means that the emission spectrum of a semimagnetic semiconductor should have a peak at energies approximately $|E_1|$ less than the band gap. The emission intensity should fall off with the temperature in accordance with (38). Experimentally, peaks in the photoluminescence of semimagnetic semiconductors have been observed in several places[10] at energies slightly below the width of the band gap. These peaks have been interpreted in those studies as resulting from the existence of excitons or impurity levels. We would pin our hopes for an experimental test of our interpretation of the photoluminescence peaks on an observation of the specific temperature dependence of the photoluminescence decay [see (38)].

States in the peaks in the band tails might be seen as attachment levels in photoconductivity. A distinguishing feature of such levels would be the temperature dependence of their concentration, which is similar to (38).

There is another prediction, which concerns the spectrum of the magnetization which arises during exposure of a semimagnetic semiconductor to polarized light. Specifically, the magnetization should reach a maximum at photon energies which generate charge carriers directly in the peaks in the band tails. The production of charge carriers with high energies would be accompanied by a depolarization of these carriers over the time taken for their trapping in the tails. The number of carriers produced by photons with lower energies, in contrast, would be exponentially small. Recent experiments on optical magnetization[11] have indeed revealed a peak at energies a few tens of millielectron volts less than the width of the band gap.

To avoid any misunderstanding, we will point out that the nonmonotonic behavior of the density of states described above should not be seen in the optical-absorption tails during interband transitions. Such transitions can be treated in Franck–Condon approximation, since the characteristic times for spin flips are comparatively long (longer than the extreme values of the reciprocal phonon frequencies). The absorption tails are determined by fluctuations created in the absence of localized charge carriers. Since fluctuations in the concentration and the spins are independent in this case, one can assert that the energy dependence of the tails of the interband absorption would be described by expressions like (1), in which we would have to replace v^2 by $v^2 + (JS/1)^2$.

On the other hand, a peak in the tail on the density of states might be manifested in the absorption if it were occupied by carriers, as it apparently is in degenerate semimagnetic semiconductors.

We note in conclusion that the exchange interaction with fluctuations in the concentration of magnetic ions could have important effects not only for band states but also for shallow impurity states.

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