PHYSICAL REVIEW B **71**, 155203 (2005)

Ferromagnetism from localized deep impurities in magnetic semiconductors

Victor Barzykin
Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996-1200, USA

(Received 5 November 2003; revised manuscript received 3 November 2004; published 15 April 2005)

We propose that localized defects in magnetic semiconductors act as deep impurities and can be described by the Anderson model. Within this model, hybridization of *d* orbitals and *p* orbitals gives rise to a non-Ruderman-Kittel-Kasuya-Yosida (RKKY) indirect exchange mechanism, when the localized *d* electrons are exchanged through both conduction and valence bands. For semiconductors with indirect band gap the non-RKKY part of exchange integral is antiferromagnetic, which suppresses ferromagnetism. In case of direct band gap, this exchange mechanism can, under certain conditions, lead to enhancement of ferromagnetism. The indirect exchange integral is much stronger than RKKY, and can be sufficiently long range. Thus, a potentially new class of high-temperature magnetic semiconductors emerges, where doped carriers are not necessary to mediate ferromagnetism. Curie temperatures in such magnetic semiconductors are determined mostly by the interaction between localized impurities, not Zener mechanism. This effect could also be responsible for unusually high Curie temperatures in some magnetic semiconductors with direct band gap.

DOI: 10.1103/PhysRevB.71.155203 PACS number(s): 75.50.Pp, 75.30.Et, 75.30.Hx, 75.50.Dd

I. INTRODUCTION

The advantage of ferromagnetic semiconductors (FSs) as a source of spin-polarized carriers is that they can be easily integrated into semiconductor devices.[1,2] When discovered, ferromagnetism at room temperatures with full polarization of itinerant carriers will be a major breakthrough in semiconductor electronics. Most theoretical and experimental efforts have been concentrated on group III-V, IV, and II-VI-based diluted magnetic semiconductors (DMSs). These semiconductors are alloys in which some atoms are randomly replaced by magnetic atoms, such as Mn^{2+}.

Ferromagnetism in diluted magnetic semiconductors (DMSs) is thought to be well understood in terms of the so-called *p-d* exchange model, which was first considered over 50 years ago.[3–5] (See also Refs. 6–8 for a review.)

At concentrations of impurities above the Mott limit, i.e., as soon as carriers become delocalized, a conventional model of FS is fairly simple. According to, for example, Ref. 5, the interaction between charge carriers in a semiconductor and spin-S impurities can be written as

$$U = -\int \mathbf{s}(\mathbf{r}) \sum_i \mathbf{S}_i J^{pd}(\mathbf{r}-\mathbf{R}_i) d^3\mathbf{r}, \tag{1}$$

where $\mathbf{S}_i$ and $\mathbf{R}_i$ are the spin and the position of an ith atom of magnetic impurity. Since the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction between the localized spins, which follows from the *p-d* model Eq. (1), has a large range, this model can usually be treated in the mean-field approximation[5]

$$U = -J^{pd}_{\mathbf{q}=0} \mathbf{s} \sum_i \mathbf{S}_i, \tag{2}$$

where $\mathbf{S}_i$ and $\mathbf{R}_i$ are the spin and the position of an ith atom of magnetic impurity, $J^{pd}_{\mathbf{q}=0} = \int J(\mathbf{r}) d^3\mathbf{r}$, and we have used the fact that magnetic impurities are randomly distributed in the sample. A simple analysis[5] then shows that, in the presence of one type of charge carriers, Curie temperature T_c is proportional to concentration of magnetic impurities N_i and the square of the strength of the exchange interaction J_{pd}:

$$T_c = \frac{n_i S(S+1)(J^{pd}_{\mathbf{q}=0})^2 \chi_0}{12\mu_0^2}. \tag{3}$$

Here μ_0 is the magnetic moment of charge carriers and χ_0 is the Pauli term in the spin susceptibility in the absence of impurities. At sufficiently large carrier densities, the spin polarization of the charge carriers at $T=0$ is given by

$$s = \frac{n_i J^{pd}_{\mathbf{q}=0} S \chi_0}{4\mu_0^2}. \tag{4}$$

In general, for any carrier density, the spin polarization is given by Zeèman-split Fermi surface, with the difference in chemical potentials for "up" and "down" spins given by

$$\mu_\uparrow - \mu_\downarrow = J^{pd}_{\mathbf{q}=0} n_i S. \tag{5}$$

The spin polarization at any filling is then very easily calculated from this equation. For example, when the carrier density

$$n_e \leqslant n_c = \frac{(2J^{pd}_{\mathbf{q}=0} n_i S m^*)^{3/2}}{6\pi^2}, \tag{6}$$

the carriers will be fully polarized at $T=0$. When $n_e > n_c$, they are no longer fully polarized. The polarization of carriers is then determined by a parametric equation (with μ as a parameter):

$$s = \frac{1}{2}(n_{e\uparrow} - n_{e\downarrow}), \tag{7}$$

where

$$n_{e\uparrow,\downarrow} = \frac{(2m^*\mu \pm J^{pd}_{\mathbf{q}=0} n_i S m^*)^{3/2}}{6\pi^2} \tag{8}$$

and $n_e = n_{e\downarrow} + n_{e\uparrow}$.

Despite the simplicity of the basic concept of Zener ferromagnetism, calculations of T_c for real materials become rather involved, and depend crucially on details of the band structure, the *p-d* exchange matrix, or direct antiferromagnetic exchange between Mn^{2+} spins. Most theoretical and experimental efforts on magnetic semiconductors have been concentrated on finding a new DMS-based material that would have a ferromagnetic transition above room temperature, and would be possible to incorporate in thin film form with mainstream semiconductor device materials. There are theoretical predictions for T_c's above room temperatures in several classes of these materials.[9,10] However, experiments indicate that the growth of Curie temperature with concentration of magnetic impurities saturates at 5–10 % Mn doping in most ferromagnetic semiconductors; it may even start to decrease at higher concentrations of Mn. Since, according to the mean field *p-d* model, the Curie temperature Eq. (3) grows linearly or faster (if the carrier concentration changes) with the growth of Mn concentration, it is important to understand what limits the growth of T_c, and how this can be avoided.

Experimental effort in FS concentrated mostly on $\mathrm{In}_{1-x}\mathrm{Mn}_x\mathrm{As}$ ($T_c \simeq 35$ K),[11] $\mathrm{Ga}_{1-x}\mathrm{Mn}_x\mathrm{As}$ ($T_c \simeq 110$ K),[12–15] and $\mathrm{Mn}_x\mathrm{Ge}_{1-x}$ ($T_c \simeq 116$ K).[16] Recently, Curie temperatures of $T_c \simeq 150$ K,[17] and even as high as $T_c \simeq 159$ K (Ref. 18) in films $\mathrm{Ga}_{1-x}\mathrm{Mn}_x\mathrm{As}$ were achieved by careful control of annealing. Dramatically higher temperature was ascribed to diffusion of Mn interstitials towards the surface.[18] While room-temperature ferromagnetism in FS remains a theoretical possibility, it is evident that the growth of T_c with increased Mn concentration slows, and even saturates. This property is quite surprising, since it is not expected from a simple mean-field treatment of the *p-d* model. It remains the focus of theoretical interest, with many plausible scenarios proposed in the literature. Originally, the saturation of T_c was ascribed to increased disorder.[13] Disorder effectively introduces an exponential cutoff for the RKKY interaction and reduces its range. Another possible reason is that the strength of direct antiferromagnetic exchange grows as the average distance between impurities becomes shorter, which, in turn, lowers the Curie temperature. Room temperature ferromagnetism has been observed in a number of compounds with *large* concentration of Mn impurities (see Ref. 2 for a review), or, due to phase separation and formation of nanoclusters of these compounds (such as $\mathrm{Mn}_{11}\mathrm{Ge}_8$ in Ref. 16). However, large carrier concentration in these compounds limits the degree of spin polarization that is necessary for device applications.

A number of different models have been proposed in the literature as plausible explanations for the observed complexity in FS. Some theoretical studies[19–21] claimed that the reason Curie temperature cannot get higher above certain concentration of Mn is that the *p-d* model cannot be treated in the mean field approximation. It was suggested in these studies that both the *p-d* interaction and disorder in high-T_c Mn-based FS are too strong to be treated perturbatively, and should be treated instead with dynamical mean field theory. The analytical and numerical results which follow from this approach show saturation of Curie temperature. Other theoretical studies[22,23] have shown that fluctuation corrections to mean field theory reduce T_c, an effect especially dramatic at higher concentrations of Mn. It has also been shown[24] that ferromagnetic phase in presence of disorder and quantum fluctuations becomes unstable against noncollinear ferromagnetic state. Recently, Zarand and Janko[25] have pointed out that due to large spin-orbit coupling in magnetic semiconductors the interaction is highly anisotropic, and thus the zero-temperature ground state remains intrinsically spin disordered. In another work Kaminski and Das Sarma[26,27] have claimed that ferromagnetic interaction and percolation of bound magnetic polarons is crucial for understanding the physics of magnetic semiconductors. All these explanations are quite plausible, and may or may not be applicable to $\mathrm{Ga}_{1-x}\mathrm{Mn}_x\mathrm{As}$ and other magnetic semiconductors. Unfortunatly, due to the complexity of the real materials (strong interactions and strong disorder), all of these effects could be playing a role in limiting the T_c.

In this paper we follow a more traditional approach, which works extremely well for other, lower T_c DMSs.[6–8,28] We adopt the idea that the mean field treatment in absence of strong disorder is justified because of the large radius of the RKKY interaction,[29] and that the reason for the discrepancy between mean field treatment of the *p-d* model and experiment lies in the presence of additional interactions in the effective spin Hamiltonian of the problem. The main objective of this paper is to consider such additional interactions theoretically, and look for conditions that make these interactions work to increase T_c rather than decrease it.

To derive effective spin Hamiltonian, including additional interactions, we start from a more general Anderson model of deep magnetic impurities in FS. We show that, in case of a deep Anderson impurity in a semiconductor, an additional long-range indirect exchange interaction appears in the effective Hamiltonian, which, if antiferromagnetic, severely limits T_c's in these materials. On the other hand, under some conditions, this interaction could be ferromagnetic. As a result, ferromagnetic correlations would become enhanced, not reduced, as the concentration of magnetic impurities grows, and high-temperature ferromagnetism could be possible even without carriers.

The indirect exchange between two deep impurities, whether ferromagnetic- or antiferromagnetic, is stronger than the RKKY interaction, and thus could produce large Curie temperatures. For example, it could provide a possible explanation of high-temperature weak ferromagnetism[30] in $\mathrm{La}_x\mathrm{Ca}_{1-x}\mathrm{B}_6$ or recently discovered $\mathrm{CaB}_2\mathrm{C}_2$ (Ref. 31) ($\mathrm{CaB}_2\mathrm{C}_2$ has $T_c = 770$ K and $M = 10^{-4}\mu_B$). Experiment[31,32] indicates that these materials are direct band semiconductors with a relatively small band gap, and that impurities play a major role in establishing the new high-temperature ferromagnetic state. However, other reports[33] claim that high-temperature ferromagnetism in these materials is not a bulk effect. Rather, it is related to clustering or new boron phases with Fe or Ni magnetic impurities. These effects are also known to appear in older FS, such as Eu chalcogenides or chromium spinels.[28] Understanding the mechanism of ferromagnetism in these materials could lead to a discovery of more members of this class of FS, where ferromagnetism is not necessarily carrier driven.

This paper is organized as follows. In Sec. II we discuss the general procedure of the derivation of the effective low-energy Hamiltonian for Anderson impurities. In Sec. III we discover that, due to strong hybridization, an Anderson impurity is no longer a local center; its localized wave function acquires a finite range, which is directly related to the corresponding "Bohr" radius of a charged impurity. Sections IV and V are devoted to the derivation of the effective exchange Hamiltonian for magnetic impurities. In Sec. VI we explore the consequences of the large range of interaction for magnetism, such as a high Curie temperature in case of a direct band gap if magnetic impurities are dense enough. In Sec. VII we consider a minor modification of the effective Hamiltonian in case of higher spin (such as $S=5/2$ for Mn), and the application of these ideas to $\mathrm{Ga}_{1-x}\mathrm{Mn}_x\mathrm{As}$. In Sec. VIII the influence of weak disorder and interactions on Curie temperature is briefly discussed. Section IX provides a summary and conclusions.

II. THE EFFECTIVE HAMILTONIAN

We start by considering a simple model of FS. In III-V systems, such as $\mathrm{Ga}_{1-x}\mathrm{Mn}_x\mathrm{As}$, it is well established that the Mn ions substitute for Ga, and contribute itinerant holes to the GaAs valence band. Experimentally, the hole density is typically a small fraction (15% or so) of the Mn concentration, perhaps due to strong localization of carriers on Mn and other defects, so $\mathrm{Ga}_{1-x}\mathrm{Mn}_x\mathrm{As}$ can be considered partially compensated. The Mn ion has a half-filled *d* shell, which acts similar to a spin-5/2 local moment. The Anderson model, which is more general than the *p*-*d* model, should completely account for all the physics of FS. It is well known that, when spins are well localized, the single-impurity Anderson Hamiltonian is reduced to the *p*-*d* Hamiltonian by the Schrieffer-Wolff transformation.[34] For many impurities, this may no longer be the case. Let us start by considering a single-orbital Anderson Hamiltonian

$$H = H_0 + H_V, \tag{9}$$

where

$$H_0 = \sum_{\mathbf{p}\sigma i} \epsilon_i(p) a^{\dagger}_{i\mathbf{p}\sigma} a_{i\mathbf{p}\sigma} + \sum_{n} \left[\epsilon_0 \sum_{\sigma} d^{\dagger}_{n\sigma} d_{n\sigma} + U d^{\dagger}_{n\uparrow} d^{\dagger}_{n\downarrow} d_{n\downarrow} d_{n\uparrow} \right]. \tag{10}$$

Here the first sum ($\mathbf{p}$) is taken over the reciprocal space, the second sum (n) over real space impurity sites. U is the on-site Coulomb repulsion term. Typically, U is very large (~ 5 eV), and can be taken to be infinite. Here $\epsilon_i(p)$ are the energy band spectra of conduction and valence bands ($i=1,2$).

The hybridization term in the model Hamiltonian H_V accounts for the *p*-*d* hybridization between impurity sites and conduction and valence bands:

$$H_V = \frac{1}{N^{1/2}} \sum_{\mathbf{p}n\sigma i} V_{\mathbf{p}i} \{ a^{\dagger}_{\mathbf{p}\sigma i} d_{n\sigma} e^{-i\mathbf{p}\cdot\mathbf{R}_n} + \mathrm{H.c.} \}. \tag{11}$$

This model is a reasonable generalization of the *p*-*d* exchange Hamiltonian, usually considered in the literature. Because of large on-site Coulomb repulsion, the *d* levels are half filled. While we consider the case of a single *d* orbital, a generalization to $S=5/2$ Mn ion is straightforward (see Sec. VII below).

The Anderson Hamiltonian (9) describes a very complicated problem. However, under the $U=\infty$ constraint, it can be reduced to the problem of Heisenberg spins (in case of a single *d* orbital, spin 1/2). The low-energy effective Hamiltonian is equivalent to Eq. (9) in the limit $k_B T \ll \Delta_i$, where Δ_i is the energy difference between the impurity *d* level and the top of the valence band, or the energy difference between the impurity *d* level and the bottom of conduction band. Since typical gap values in semiconductors are of the order of 1 eV, this is usually a valid assumption.

Following Refs. 35 and 36, the effective spin Hamiltonian can be derived by expanding the *S* matrix (or, at finite temperatures, the partition function) in *V*'s, and reexpressing various time-ordered processes in terms of spin operators. Then, these processes are collected back under exponent, to obtain the effective Hamiltonian. This method allows one to obtain consistently the interaction between spins and carriers (electrons or holes) in conduction and valence bands, and carrier-carrier interaction. In a way, the concept is similar to perturbative renormalization group, since we arrive at a low-energy effective Hamiltonian by integrating out higher-energy states. Treating hybridization term in Eq. (9) as a perturbation, we can rewrite the partition function as

$$Z = \mathrm{Tr}[\exp(-\beta H_0) S(\beta)], \tag{12}$$

where

$$\begin{aligned} S(\beta) &= T \exp\left(- \int_0^{\beta} H_V(\tau) d\tau \right) \\ &= T \exp\left(- \sum_{n\sigma i} \int_0^{\beta} d\tau V_i \{ \Psi^{\dagger}_{n\sigma i}(\tau) d_{n\sigma}(\tau) \right. \\ &\quad \left. + d^{\dagger}_{n\sigma}(\tau) \Psi_{n\sigma i}(\tau) \} \right). \end{aligned} \tag{13}$$

The problem of finding the effective Hamiltonian is then to reduce these expressions to the form

$$Z = \mathrm{Tr}(\exp[-\beta H_{\mathrm{eff}}]), \tag{14}$$

using the $k_B T \ll \Delta_i$ condition, i.e., the fact that the local levels are almost always occupied, and that transitions to conduction and valence bands are absent at low temperatures. Various terms in the effective Hamiltonian can then be associated with certain time-ordered virtual processes. For example, the first nonzero contribution to H_{eff} is from the second order term in the expansion of Eq. (13) in V_i:

$$S_2(\beta) = \sum_{n\sigma\sigma'} V_1^2 \int_0^{\beta} d\tau_1 \int_{\tau_1}^{\beta} d\tau_2 \Psi_{n\sigma 1}(\tau_2) \Psi^{\dagger}_{n\sigma' 1}(\tau_1) d^{\dagger}_{n\sigma}(\tau_2) d_{n\sigma'}(\tau_1). \tag{15}$$

The order of operators $d^{\dagger}_{n\sigma}(\tau_2) d_{n\sigma'}(\tau_1)$ $(\tau_2 > \tau_1)$ is fixed by the assumption of strong Coulomb repulsion on the *n*th center. Note that, in the second order, because all centers are filled, only one band contributes to the effective Hamiltonian. The "filled" band does not contribute, because of the Pauli principle (this is not the case at a finite *U*). The pertur-

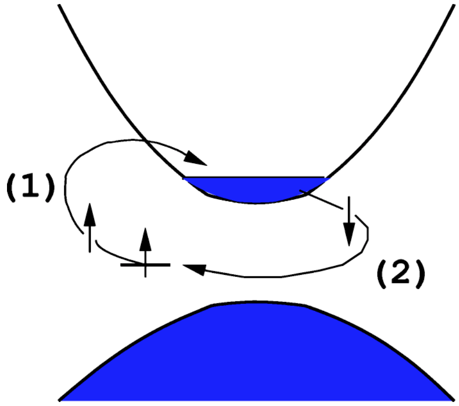

FIG. 1. The second-order contribution to the effective Hamiltonian, shown as a time-ordered process.

bative time-ordered process corresponding to the term in Eq. (15) is shown in Fig. 1.

We may rewrite $\Psi_{n\sigma 1}(\tau_2)\Psi^{\dagger}_{n\sigma' 1}(\tau_1)$ in the interaction representation as

$$\Psi_{n\sigma 1}(\tau_2)\Psi^{\dagger}_{n\sigma' 1}(\tau_1) = \{\Psi_{n\sigma 1}(\tau_2)\Psi^{\dagger}_{n\sigma' 1}(\tau_1)\}_{+} - \Psi^{\dagger}_{n\sigma' 1}(\tau_1)\Psi_{n\sigma 1}(\tau_2). \tag{16}$$

The first term in Eq. (16) is a c number. In the limit $\Delta_1 \gg k_B T$ it is possible to put $\tau_1 \simeq \tau_2$ in the second term in Eq. (16). Thus, for the second-order contribution in the effective Hamiltonian we may written

$$H^{(2)}_{\text{eff}} = -\sum_{\mathbf{p}} \frac{V^2_{\mathbf{p}1}}{\epsilon_{1p} - \epsilon_0} + \frac{V^2_{\mathbf{p}_0 1}}{\Delta_1} \sum_{n\sigma\sigma'} \Psi^{\dagger}_{n\sigma' 1}\Psi_{n\sigma 1}\left(\frac{1}{2}\delta_{\sigma\sigma'} + \mathbf{S}_n \sigma_{\sigma'\sigma}\right), \tag{17}$$

where $\mathbf{S}_n$ is the localized spin of the nth impurity and $\mathbf{p}_1$ is the location of the bottom of the band 1 in momentum space. The first term corresponds to the renormalization of the energy of the localized level, while the second term involving spins of localized impurity and carriers is nothing but the ordinary H_{pd}, the p-d model discussed in Sec. I.

The next order terms in the effective Hamiltonian are fourth order in V's. There are sums over two local centers, m and n in $S_4(\beta)$. Also, there are contributions to $S_4(\beta)$, which we will denote $S'_4(\beta)$, that are already accounted for in the effective Hamiltonian (17):

$$S'_4(\beta) = \frac{1}{2}\int\int d\tau_1 d\tau_2 T\{H_{pd}(\tau_1)H_{pd}(\tau_2)\}. \tag{18}$$

These contributions need to be subtracted from $S_4(\beta)$, to get the fourth-order (in V_i) contributions in the effective Hamiltonian. The most important contribution is the effective exchange interaction between localized spins:

$$H^{(4)}_{ex} = -\sum_{n\neq m} J(\mathbf{R}_n - \mathbf{R}_m)\mathbf{S}_n \cdot \mathbf{S}_m \tag{19}$$

This exchange interaction is the result of two time-ordered processes shown in Figs. 2 and 3. One is the superexchange (Fig. 2), which is a result of the localized spins exchanged through the empty conduction band. The other process is the Bloembergen-Rowland term[37] (Fig. 3), an exchange process through both conduction and valence bands. The form of these contributions will be discussed in greater detail in Secs. IV and V below.

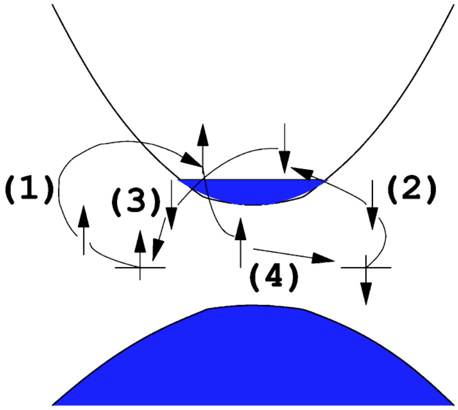

FIG. 2. The fourth-order antiferromagnetic superexchange contribution to the effective exchange interaction between two localized impurities.

In addition, other interesting contributions arise as a result of fourth-order processes, such as p-d scattering by spins on two centers

$$H^{(4)}_{pd2c} = \frac{V^2_{\mathbf{p}_1 1}}{\Delta^2_1} \sum_{n\neq m,\sigma\sigma'} t(\mathbf{R}_n - \mathbf{R}_m)\Psi^{\dagger}_{m\sigma' 1}\Psi_{n\sigma 1}[\mathbf{S}_n \cdot \mathbf{S}_m \delta_{\sigma'\sigma} + i([\mathbf{S}_m \cdot \mathbf{S}_n]\hat{\sigma}_{\sigma'\sigma})], \tag{20}$$

nontrivial local contribution

$$H^{(4)}_{\text{local}} = -\frac{V^4_{\mathbf{p}_1 1}}{\Delta^3_1} \sum_{n\sigma\rho\rho'} \Psi^{\dagger}_{n\sigma 1}\Psi^{\dagger}_{n\rho' 1}\left[\frac{1}{2}\delta_{\rho'\rho} + (\hat{\sigma}_{\rho'\rho}\mathbf{S}_n)\right]\Psi_{n\rho 1}\Psi_{n\sigma 1}, \tag{21}$$

and corrections to the energy of the local level and ground state energy, which are dropped. These nontrivial terms, however, are higher order in carrier density, which is small in

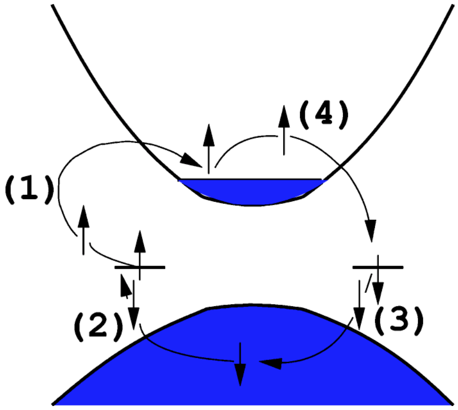

FIG. 3. The fourth-order Bloembergen-Rowland term in the effective exchange interaction.

magnetic semiconductors. Thus, they don't play any significant role in magnetism, and, hence, will not be discussed in any detail. We refer the reader to Refs. 35, 36, and 38, where these terms were discussed in detail in connection with the three-band model of cuprate superconductors (see also Refs. 28 and 39).

III. RENORMALIZATION OF LOCAL LEVEL DUE TO HYBRIDIZATION

To clarify the new physics of an Anderson impurity, in comparison with *p-d* magnetic impurity, let us first consider a single-level problem ($\mathbf{R}_n=0$), interacting only with the conduction band (i.e., we take $V_2=0$ for simplicity). The Hamiltonian is defined on the manifold of wave functions $\{\Phi_0, \Psi_{1\mathrm{p}_1}, \Psi_{1\mathrm{p}_2}, \ldots\}$, which correspond to the exact solution for a center in crystalline lattice in the absence of hybridization. These wave functions form a complete orthogonal basis for the single-particle problem. We may now introduce the hybridization as a perturbation into the Schrödinger equation. In the matrix representation, the single-level Hamiltonian takes a very simple form

$$H = \left\{ \begin{array}{cccc} \epsilon_0 & v_{\mathbf{p}_1 1} & v_{\mathbf{p}_2 1} & \cdots \\ v_{\mathbf{p}_1 1} & \epsilon_{1\mathbf{p}_1} & 0 & \cdots \\ v_{\mathbf{p}_2 1} & 0 & \epsilon_{1\mathbf{p}_2} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{array} \right\}. \tag{22}$$

Here $v_1 \equiv V_1/N^{1/2}$. This Hamiltonian can be easily diagonalized, by looking for a solution for the ground state wave function as a linear combination of all single-particle states

$$\Psi = \chi_0 \Phi_0 + \sum_{\mathbf{p}} \{\chi_{\mathbf{p}}^{(1)} \Psi_{1\mathbf{p}}\}, \tag{23}$$

where the coefficients obey the following set of equations:

$$(\epsilon_0 - \epsilon)\chi_0 + \sum_{\mathbf{p}} v_{\mathbf{p}1}\chi_{\mathbf{p}} = 0, \tag{24}$$

$$v_{\mathbf{p}1}\chi_0 + (\epsilon_{1\mathbf{p}} - \epsilon)\chi_{\mathbf{p}} = 0.$$

Solving Eq. (24) gives the new position of the localized level

$$\epsilon = \epsilon_0 - \frac{1}{N}\sum_{\mathbf{p}} \frac{V_{\mathbf{p}1}^2}{\epsilon_{1\mathbf{p}} - \epsilon}. \tag{25}$$

Thus, in presence of hybridization the position of the impurity level is shifted. If the depth of the level $\Delta_1 \ll D_1$, where D_1 is the bandwidth of the conduction band (which is usually a valid assumption for semiconductors, where the band gap is much smaller than the corresponding bandwidths of conduction and valence bands), the sum in Eq. (25) can be performed numerically. The correction to the energy level

$$\epsilon - \epsilon_0 \sim \frac{V_1^2}{D_1} \tag{26}$$

turns out to be small for small enough hybridization parameter $V_1 \ll \sqrt{D_1\Delta_1}$. It is responsible for a slight downward shift of the energy level. Such corrections will thus be dropped in our further discussion.

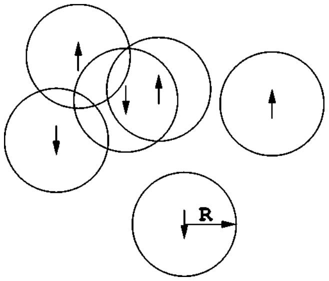

FIG. 4. Localized centers acquire a finite radius in the Anderson model. This radius can be as large as 2–3 lattice spaces in magnetic semiconductors. An overlap of wave functions from two localized level leads to the new physics, which is not captured by the traditional *p-d* model.

The wave function of the localized level, according to Eq. (24), acquires an admixture to its decay in the form

$$\delta\Phi_0(r) \sim V_{\mathbf{p}_1 1} m_1 a^2 \frac{a}{r} e^{-r\sqrt{2m_1\Delta_1}}. \tag{27}$$

Here a is the lattice constant (we assume a simple cubic lattice), m_1 is the effective mass of carriers in the empty band (for hole-doped materials, the valence band is the "empty" band, since it is empty of holes), Δ_1 is the energy difference between impurity levels and the bottom of the empty band, $\mathbf{p}_1$ is the location of the bottom of the empty band in momentum space. Thus, a new length scale enters the problem

$$R_0 = (2m_1\Delta_1)^{-1} \sim a\sqrt{D_1/\Delta_1}, \tag{28}$$

which, while small compared to the average distance between doped carriers, may considerably exceed interatomic distances (the large parameter is the square root of the ratio of the bandwidth to the energy gap in a semiconductor), and become comparable to the average distance between magnetic impurities. The overlap of the localized wave functions gives rise to a new contribution to the exchange integral, which will be derived below. The picture of finite-radius localized magnetic impurities with overlapping wave functions is shown in Fig. 4.

Existence of a large (compared to lattice spacing) radius for deep impurities was first noticed by Keldysh,[40] who analyzed deep charged impurities in ordinary semiconductors. In his case, however, this scale corresponded to ordinary Bohr radius for a deep impurity (modified by the fact that in that case one had to consider Dirac Hamiltonian for the *k-p* model of semiconductors). In our case, the large length scale comes from the hybridization of the localized impurity level with conduction and valence bands. We will also see below in Sec. VI that effective length scale, at which direct interaction between impurities starts to matter, grows logarithmically with decreasing temperature in the framework of percolation theory or virial expansion. Thus, at low temperatures, such as Curie temperature, the effective range of interaction between two impurities becomes even larger.

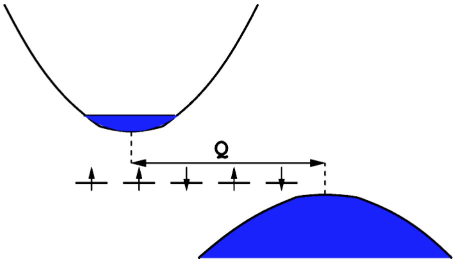

FIG. 5. Positions of conduction and valence bands.

IV. THE EXCHANGE HAMILTONIAN

The problem of magnetism in the Anderson model can be reduced to the spin Hamiltonian (19), described by the processes shown in Figs. 2 and 3. In case when the empty band (the "empty" band can also be the valence band, in case of hole doping) gets partially filled by carriers (electrons or holes), the time-ordered processes shown in Figs. 2 and 3 include all possible contributions—the familiar RKKY exchange interaction, the superexchange, and the Bloembergen-Rowland interaction. In presence of carriers, the superexchange gets modified by the RKKY exchange term. We shall see below, that the Bloembergen-Rowland interaction also gets modified in presence of dopants. This modification is not accounted for by the RKKY interaction. As we have discussed in the previous section, localized impurities in the Anderson model acquire a large radius (compared with the lattice constant a). Thus, exchange interaction between localized spins is, in general, long range. This would allow one to use mean-field to describe the ferromagnetic ordering, if the concentration of localized spins is high enough. On the other hand, if the concentration of magnetic impurities is low, one can use percolation theory or virial expansion.

Let us first consider exchange integrals given by the processes shown in Figs. 2 and 3 for a semiconductor with conduction and valence bands separated by some general reciprocal space wave vector $\mathbf{Q}$, as shown in Fig. 5. When $\mathbf{Q}=0$, it is a direct band gap semiconductor. Surprisingly, all exchange processes can be written in a relatively compact way:

$$J(R) = \sum_{i,j} J_{ij}(R), \tag{29}$$

where

$$J_{ij} = 2\frac{a^6}{(2\pi)^6}\int d^3\mathbf{p}\,d^3\mathbf{q}\,\frac{|V_{\mathbf{p}i}|^2|V_{\mathbf{p+q}j}|^2[1-n(\epsilon_{\mathbf{p}i}-\mu)]e^{i\mathbf{q}\cdot\mathbf{R}}}{(\epsilon_{\mathbf{p}i}-\epsilon_{\mathbf{p+q}j})(\epsilon_{\mathbf{p}i}-\epsilon_0)^2}. \tag{30}$$

Here i,j are the band indices for conduction and valence bands, μ is the chemical potential, and $n(\epsilon-\mu)$ is the Fermi-Dirac distribution function. The empty band corresponds to $i=1$, while the filled band has the band index $i=2$. We can see now, that for $T \ll \Delta_0$, where Δ_0 is the band gap, the contributions J_{21} and J_{22} are absent. J_{11} is the superexchange, which corresponds to the process shown in Fig. 2. In presence of carriers, this process, and the corresponding expression, also includes the RKKY contribution. When carriers are present, the effective Hamiltonian can be written in terms of impurity spins only, with carriers "integrated out." In this case, impurity spins interact with the exchange Hamiltonian (29) and (30), which includes RKKY. If, however, we wish to retain carriers, and the carrier-impurity *p-d* exchange interaction, as we described in Sec. II, then the RKKY part will be the part $S'(\beta)$ in the fourth order [see Eq. (18)], which has to be subtracted, and the indirect exchange interaction will be described by Eq. (30) at zero doping, i.e., with the factor $[1-n(\epsilon_{\mathbf{p}i}-\mu)]$ in Eq. (30) replaced by 1. These two descriptions are only equivalent when the chemical potential for doped carriers $\mu \ll \Delta_1$. Basically, when the doped carriers are retained, we "integrate out" electrons and holes in the original Anderson Hamiltonian up to the scale μ. When we consider the Hamiltonian for localized spins only, we integrate out all carriers. It makes sense to define the RKKY interaction for the Anderson model as the difference between the doped and undoped cases in Eqs. (29) and (30). When $\mu \sim \Delta_1$, the Anderson model *cannot* be reduced to the *p-d* model, except near the Fermi surface. The Anderson model expression for the RKKY interaction in real space will then *differ* from the corresponding *p-d* model expression at *short* distances, which are important for ferromagnetism. We will not consider this subtle point any further, since we will always assume the carrier density in FS to be small, i.e., $\mu \ll \Delta_1$. In this section and the next section we will deal with an effective Hamiltonian for spins only, i.e., when all carriers are integrated out. This procedure for the Anderson model is always justified (although, as we commented above, a reduction to the *p-d* model is *not*). J_{12} is the Bloembergen-Rowland interaction, which also gets somewhat modified by doped carriers. Note that the expression for the exchange integral (30), obtained from the Anderson model, differs from the original expression of Bloembergen and Rowland;[37] it includes the term $(\epsilon_{\mathbf{p}1}-\epsilon_0)^2$ in the denominator, which makes the exchange integral in the Anderson model long range. The final result of Bloembergen and Rowland is erroneous, since the Brillouin zone in their calculations was replaced by a sphere, and the spatial dependence of Bloch amplitudes was neglected.[41] The short-distance behavior thus has to be calculated from the band structure. Nevertheless, the Bloembergen-Rowland interaction was shown to be important at large distances, where its behavior can be obtained analytically.[41] In this paper, we also consider long-range behavior of the Bloembergen-Rowland interaction. Thus, concerns about the errors in the original Bloembergen-Rowland calculation also do not apply. The hybridization parameters $V_{\mathbf{p}i}$ account for the Bloch amplitudes. Finally, we note that while the physics of J_{12} is similar to the Bloembergen-Rowland interaction, it, unlike RKKY, does not appear as a result of the second order (in V's) terms in the effective Hamiltonian, but rather appears directly in the fourth order. This difference accounts for different asymptotic behavior obtained below for J_{12} from that of the Bloembergen-Rowland interaction.[41]

Both contributions to exchange integral can be evaluated analytically when $\Delta_1 \ll D$, since the dominant contribution to the integral over the momenta is coming from the bottom of the conduction band and the top of the valence band. Due to this condition, the exchange integral becomes long range

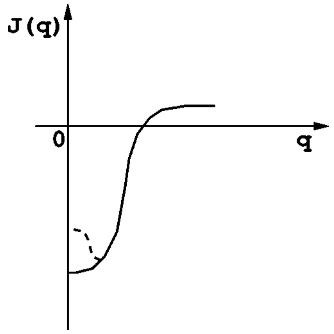

FIG. 6. Superexchange contribution to exchange integral in q space; modification by RKKY in presence of carriers is shown by a dotted line.

compared to lattice spacing. When $\Delta_1 \sim D$, numerical approach is required. These contributions are shown schematically in Figs. 6 and 7.

We see that the superexchange is, in general, antiferromagnetic, while the Bloembergen-Rowland contribution favors a spin density wave with a wave vector $\mathbf{Q}$, separating conduction and valence bands. Both exchange processes are, in general, of the same order, and their relative strength is determined by the corresponding hybridization parameters V_1 and V_2. The superexchange integral in the $\mathbf{q}$ space, in the absence of carriers, can be easily found analytically

$$J_{11}(\mathbf{q}) = -\frac{2V_1^4 a^3 m_1^3}{\pi\sqrt{2m_1\Delta_1}} \frac{1}{q^2 + 8m_1\Delta_1}. \tag{31}$$

Since $V_{\mathbf{p}i}$ vary slowly over the Brillouin zone, while the expression under the integral is highly peaked, their value can be approximately taken at momenta for the bottom of the conduction band (and the top of the valence band). Thus, we will drop the momentum index in $V_{\mathbf{p}i}$'s from all the expressions obtained further in this section and Sec. V, meaning that

$$V_i \equiv V_{\mathbf{p}_i, i}, \tag{32}$$

where $\mathbf{p}_i$ are the locations of the bottom of the conduction band i or top of the valence band i in momentum space. In presence of carriers, $J_{11}(\mathbf{q})$ gets modifed by the RKKY interaction

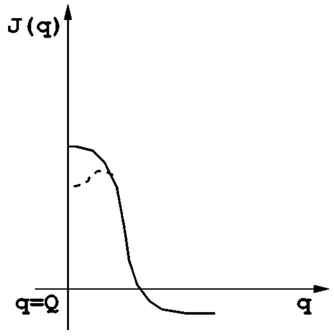

FIG. 7. Bloembergen-Rowland contribution to exchange integral in q space; modification in presence of carriers is shown by a dotted line.

$$\delta J_{11}(\mathbf{q}) \equiv J_{\mathrm{RKKY}}(\mathbf{q}) = \frac{V_1^4 a^3 m_1 p_F}{(2\pi)^2 \Delta_1^2} \times \left\{ 1 + \left(\frac{p_F}{q} - \frac{q}{4p_F} \right) \ln \left(\frac{1 + \frac{q}{2p_F}}{1 - \frac{q}{2p_F}} \right) \right\}, \tag{33}$$

where $p_F = \sqrt{2m_1\mu}$ is the Fermi momentum for doped carriers. The superexchange and RKKY contributions can be easily rewritten in real space:

$$J_{11}(R) = J_{se}(R) + J_{\mathrm{RKKY}}(R), \tag{34}$$

with

$$J_{se}(R) = -\frac{V_1^4 a^6 m_1^3}{2\pi^2\sqrt{2m_1\Delta_1}R} \exp\{-\sqrt{8m_1\Delta_1}R\}, \tag{35}$$

and a standard expression for the RKKY interaction, taking into account that $J_{pd} \equiv 2V_1^2/\Delta_1$ [note that in Eq. (19) we sum over each pair of impurities twice]:

$$J_{\mathrm{RKKY}}(R) = -J_{\mathrm{RKKY}} F(2p_F R), \tag{36}$$

where

$$F(x) = \frac{\cos(x)}{x^3} - \frac{\sin x}{x^4}, \tag{37}$$

and

$$J_{\mathrm{RKKY}} = \frac{V_1^4 a^6 m_1 p_F^4}{\pi^3 \Delta_1^2}. \tag{38}$$

We define the RKKY interaction in the Anderson model formulation as the difference between $J_{11}(R)$ in doped and undoped cases, given by Eq. (30). As we emphasized above, since it depends explicitly on impurity energy level, when $\Delta_1 \sim \mu$, this expression differs from the usual RKKY form. Its asymptotic behavior at large distances, certainly, does not change. In what follows we assume that the carrier concentration is always low $\mu \ll \Delta_i$, so that $J_{\mathrm{RKKY}}(R)$ is given by the standard expression. Note that if J_{pd} and the level position are known, the exchange integral (34) contains no free parameters:

$$J_{11}(R) = -J_{\mathrm{RKKY}} \left(F(2p_F R) + \frac{\pi(m_1\Delta_1)^{3/2}}{2\sqrt{2}p_F^4 R} e^{-2\sqrt{2m_1\Delta_1}R} \right). \tag{39}$$

Similar to superexchange, the Bloembergen-Rowland interaction can also be written in two parts. The first part is from the empty and filled bands, while the second part takes doped carriers into account:

$$J_{12}(\mathbf{q}) = J_{\mathrm{BR}}(\mathbf{q}) + J'_{12}(\mathbf{q}). \tag{40}$$

The first contribution in Eq. (40) favors a spin density wave with a wave vector $\mathbf{Q}$, separating conduction and valence bands, and has a rather cumbersome form

$$J_{\mathrm{BR}}(\mathbf{q}) = \frac{a^3V_1^2V_2^2m_1^2m_2}{\pi\sqrt{2m_1\Delta_1}} \times \left\{ \frac{m_1\Delta_1 + m_2\Delta_1 + \dfrac{q^2}{2} + m_2\Delta_0 - \sqrt{2(m_1+m_2)\Delta_1}\sqrt{2m_2\Delta_0 + q^2\dfrac{m_2}{m_1+m_2}}}{\Delta_1^2(m_1+m_2)^2 + \Delta_1(q^2(m_1-m_2) - 2m_2(m_1+m_2)\Delta_0) + \left(\dfrac{q^2}{2} + m_2\Delta_0\right)^2} \right\}. \tag{41}$$

Here and below in this section the notation will be slightly different; $\mathbf{q}$ is now the *difference* from $\mathbf{Q}$ (the wave vector separating the bottoms of the two bands), i.e., we change our notation in the following way: $\mathbf{q}-\mathbf{Q}\to\mathbf{q}$. In general, the Bloembergen-Rowland contribution (41) is quite cumbersome, which makes it impossible to find an explicit analytical expression in real space, except in some limiting cases. However, the leading asymptotic behavior of $J_{\mathrm{BR}}(R)$ at large distances can be derived. If the deep impurity level lies inside the gap $\Delta_1 < \Delta_0$, we find an exponential decay of exchange correlations

$$J_{\mathrm{BR}}(\mathbf{R}) \simeq \frac{a^6V_1^2V_2^2m_1m_2}{2\sqrt{2}\pi^2R} \times\left(\sqrt{\frac{m_1}{\Delta_1}} - \sqrt{\frac{m_2}{\Delta_0-\Delta_1}}\right)\cos(\mathbf{Q}\cdot\mathbf{R})e^{-R/R_1}, \tag{42}$$

where the range of the integral is

$$R_1 = \frac{1}{\sqrt{2m_1\Delta_1} + \sqrt{2m_2(\Delta_0-\Delta_1)}}. \tag{43}$$

On the other hand, when the deep impurity level enters the filled band $\Delta_1 > \Delta_0$, the Bloembergen-Rowland contribution has an oscillating decaying asymptotic

$$J_{\mathrm{BR}}(\mathbf{R}) = \frac{a^6V_1^2V_2^2m_1m_2}{\sqrt{2}\pi^2R}\left(\sqrt{\frac{m_1}{2\Delta_1}}\cos\frac{R}{R_{c1}} + \sqrt{\frac{m_2}{2(\Delta_1-\Delta_0)}}\sin\frac{R}{R_{c1}}\right)\cos(\mathbf{Q}\cdot\mathbf{R})e^{-R/R_{c0}}, \tag{44}$$

where

$$R_{c1} = \frac{1}{\sqrt{2m_1(\Delta_1-\Delta_0)}}, \quad R_{c0} = \frac{1}{\sqrt{2m_1\Delta_1}}. \tag{45}$$

The contribution from doped carriers to J_{12} can be derived as well:

$$J'_{12}(\mathbf{q}) \simeq -\frac{a^3V_1^2V_2^2p_F^3}{3\pi^2\Delta_1^2\left(\Delta_0 + \dfrac{q^2}{2m_2}\right)}. \tag{46}$$

In real space, this contribution becomes

$$J'_{12}(\mathbf{R}) \simeq -\frac{p_F^3a^6V_1^2V_2^2m_2}{6\pi^3\Delta_1^2R}\cos(\mathbf{Q}\cdot\mathbf{R})e^{-\sqrt{8m_2\Delta_0}R}. \tag{47}$$

We see that if $\mathbf{Q}=0$, i.e., when our FS has a direct band gap, the Bloembergen-Rowland mechanism gives a large ferromagnetic short-range contribution to the exchange integral. At high enough concentration of impurities, ferromagnetic properties are then determimed by the value of exchange integral at $\mathbf{q}=0$. This value can be easily written down (it is only valid for a direct band gap FS):

$$\begin{aligned} J(\mathbf{q}=0) &= J_{11}(\mathbf{q}=0) + J_{12}(\mathbf{q}=0) \\ &= \frac{2a^3V_1^2m_1^2}{\pi\sqrt{2m_1\Delta_1}}\left(-\frac{V_1^2}{8\Delta_1} + \frac{V_2^2m_2}{(\sqrt{2(m_1+m_2)\Delta_1} + \sqrt{2m_2\Delta_0})^2}\right). \end{aligned} \tag{48}$$

In this section we have derived explicitly the interaction between two magnetic impurities in a semiconductor with one conduction and one valence band. Typically, the band structure of semiconductors is more complex than that (for example, GaAs has light and heavy hole bands). This situation is considered in the next section.

V. WHAT IF A SEMICONDUCTOR HAS MORE THAN TWO BANDS?

When a semiconductor has many bands, the analysis is just as straightforward as in case of two bands considered in the previous section. The exchange integral between two impurities is still given by Eqs. (29) and (30), where the sum now goes over all pairs of band indices. The case when $i=j$ is an "empty" band index corresponds to a superexchange contribution (Fig. 2), considered in detail in the previous section; $J_{ij}=0$ when i is a "filled" band index, because of the Pauli principle; J_{ij} is the Bloembergen-Rowland contribution (Fig. 3), when i is an "empty" band index; and j is a "filled" band index. The contribution of a new type appears when one has two or more "empty" bands in a semiconductor. Then there will be a superexchange contribution of the type shown in Fig. 2, where now the carriers are exchanged through two different "empty" bands—the process (1) in Fig. 2 puts a carrier from one magnetic impurity into the first "empty" band, while the process (2) puts a carrier from the other magnetic impurity into the second "empty" band. Naturally, there are two such contributions J_{ij} and J_{ji}, where $i\neq j$ indices correspond to two different "empty" bands. The exchange Hamiltonian in any FS is a sum of all pairwise contributions listed above.

Let us now consider the new two-band superexchange contribution in detail. In the most general case, the bottom of the second "empty" band is shifted from the bottom of the first “empty” band by a wave vector **Q**. The bottoms of the two bands also lie at two different positive energies Δ_1 and Δ_2 relative to impurity level, unless there is a symmetry-related degeneracy, and the carriers in the first and second bands have different effective masses m_1 and m_2.

Let us first consider the simplified case when the bands 1 and 2 are identical (i.e., $\Delta_1 = \Delta_2$ and $m_1 = m_2$), but separated by a wave vector **Q**. Then we do not have to do the calculation, since $\epsilon_{\mathbf{p}2} = \epsilon_{\mathbf{p}-\mathbf{Q}1}$, and it can be easily seen from Eq. (30), that

$$J_{12}(\mathbf{q}) = J_{11}(\mathbf{q}-\mathbf{Q}), \tag{49}$$

and

$$J_{12}(R) = J_{11}(R)e^{i\mathbf{Q}\cdot\mathbf{R}}. \tag{50}$$

Summing all contributions from two identical empty bands, since $J_{11}(R) = J_{22}(R)$, we get

$$J_{2bse} = 2J_{11}(R)[1+\cos(\mathbf{Q}\cdot\mathbf{R})]. \tag{51}$$

This also includes RKKY-type contribution for two identical bands at finite doping, described by

$$J_{12\mathrm{RKKY}} + J_{21\mathrm{RKKY}} = 2J_{\mathrm{RKKY}}(R)\cos(\mathbf{Q}\cdot\mathbf{R}), \tag{52}$$

and the ordinary RKKY interaction from both bands. It is rather obvious from Eq. (52), that at a finite density of carriers there are ordinary one-band RKKY contributions from both bands. The two-band RKKY contribution oscillates much more rapidly in space, as $\cos(\mathbf{Q}R)$, unless $\mathbf{Q}=0$. In the latter case, the two-band RKKY contribution just enhances the contributions from the two separate bands. In the case when $\mathbf{Q}=0$, the 12 and 21 exchange integrals take the same form as shown in Fig. 6. For $\mathbf{Q}\neq 0$, these contributions have the same form in **q** space as for $\mathbf{Q}=0$, centered at the wave vector $\mathbf{q}=\mathbf{Q}$.

Now that the form of new two-band contributions to the exchange integral has become clear from the simplified case, let us consider a more general case of two completely different “empty” bands. The bottom of the second band is shifted from the bottom of the first band by the wave vector **Q**. Of course, 12 and 21 contributions to $J(\mathbf{q})$ will still be of the form shown in Fig. 6, with the bottom at $\mathbf{q}=\mathbf{Q}$, but the corresponding expressions become more combersome. Let us assume that $\Delta_1 < \Delta_2$, i.e., the bottom of the first band lies below the bottom of the second band, and the first band gets filled by carriers first. We consider three separate cases (1) both bands are empty, (2) the first band gets filled by carriers, but the second band is empty, and (3) both bands get partially filled by carriers. When $\Delta_1 = \Delta_2$, i.e., the two bands are symmetry-related, we only have cases (1) and (3). As before, we assume that the carrier concentration is very small, i.e., the Fermi energy for doped carriers is much smaller than any other energy scale in the problem, except temperature.

(1) Both bands are empty. Let us now consider the exchange interaction arising from two empty bands. The integral in Eq. (30) can be easily calculated:

$$J_{12+21}(\mathbf{q}) = -\frac{\sqrt{2}V_1^2V_2^2m_1m_2a^3}{(\mathbf{q}-\mathbf{Q})^2+(\sqrt{2m_1\Delta_1}+\sqrt{2m_2\Delta_2})^2} \times\left(\sqrt{\frac{m_1}{\Delta_1}}+\sqrt{\frac{m_2}{\Delta_2}}\right). \tag{53}$$

In the coordinate space, it takes the following form:

$$J_{12+21}(\mathbf{R}) = -V_{12}\cos(\mathbf{Q}\cdot\mathbf{R})\frac{1}{R}\exp\left(-\frac{R}{R_{12}}\right), \tag{54}$$

where the range of this interaction is given by

$$R_{12} = \frac{1}{\sqrt{2m_1\Delta_1}+\sqrt{2m_2\Delta_2}} \tag{55}$$

and

$$V_{12} = \frac{V_1^2V_2^2a^6m_1m_2}{2\sqrt{2}\pi^2}\left(\sqrt{\frac{m_1}{\Delta_1}}+\sqrt{\frac{m_2}{\Delta_2}}\right). \tag{56}$$

(2) One band gets filled. Let us assume in this section that band one gets filled first, i.e., $\Delta_1 < \Delta_2$. We also assume that the chemical potential (counted from the bottom of band one), $\mu_1 \ll \Delta_2 - \Delta_1$, i.e., the number of carriers is low. Of course, the main part of the exchange integral is still given by Eq. (54). However, at finite doping there are corrections. Obviously, since only band one gets carriers, $\delta J_{21} = 0$. At small filling, RKKY-like correction can be easily calculated:

$$\delta J_{12}(q) \simeq \frac{2V_1^2V_2^2a^3P_{F1}^3m_2}{3\pi^2\Delta_1^2(2m_2[\Delta_2-\Delta_1]+q^2)}. \tag{57}$$

Here q denotes the difference from **Q**, the wave vector separating the bottoms of the two bands. In coordinate space it can be written as

$$\delta J_{12}(\mathbf{R}) \simeq \frac{V_1^2V_2^2a^6p_{F1}^3m_2}{6\pi^3\Delta_1^2R}e^{-R/R_g}\cos\mathbf{Q}\cdot\mathbf{R}, \tag{58}$$

where

$$R_g = \frac{1}{\sqrt{2m_2(\Delta_2-\Delta_1)}}. \tag{59}$$

(3) Both bands get filled. When $\Delta_1 = \Delta_2 = \Delta$ by symmetry, both bands get filled by carriers simultaneously. The result of this is an RKKY-like correction to exchange integral (54), which is given by Eq. (52) for two identical bands. If the bands have different masses, the interaction is RKKY-like long range, but the general expression is quite messy. Here we give the its value at $\mathbf{q}=\mathbf{Q}$, which is important for ferromagnetism, when $\mathbf{Q}=0$:

$$\delta J_{12+21}(\mathbf{q}=\mathbf{Q}) = \frac{2V_1^2V_2^2a^3\sqrt{2\mu}m_1m_2}{\pi^2\Delta^2(\sqrt{m_1}+\sqrt{m_2})}. \tag{60}$$

To summarize this section, the exchange interaction in any magnetic semiconductor is composed of pairwise contributions: the superexchange contribution through one “empty” band, the Bloembergen-Rowland contribution from one “empty” and one filled band, and a pairwise contribution from two different “empty” bands. The last contribution was considered in this section. It includes two-band long-range RKKY-like interaction at finite doping, which is usually not taken into account in the p-d Hamiltonian. Note that when $\mathbf{Q} \neq 0$, the two-band RKKY interaction will favor spin glass order, *not* ferromagnetism, since it oscillates very rapidly in real space.

VI. THE MEAN-FIELD APPROXIMATION, VIRIAL EXPANSION, AND PERCOLATION

Now that we have obtained all terms in the exchange interaction (30), we can proceed to calculate magnetic properties of ferromagnetic semiconductors. In general, the RKKY exchange interaction is always long-range. The shorter-range contributions may or may not be treated in mean field, depending on the ratio of their range to the average inter-impurity distance. We assume here, for simplicity, that one of indirect exchange processes considered in the previous two sections dominates the short-range physics. In case of FS with indirect band gap, the Bloembergen-Rowland exchange contribution favors antiferromagnetism with a lattice wave vector $\mathbf{Q}$. It oscillates very rapidly in real space. Since impurities are distributed randomly, it would favor a spin glass ordering. The contributions at $\mathbf{Q}=0$, which influence ferromagnetism, are the RKKY and the superexchange. From Eq. (39) one can easily see that, when impurity concentration $n_i \gg (m_1\Delta_1)^{3/2}$, the superexchange contribution totally suppresses ferromagnetism brought about by the RKKY exchange interaction. On the other hand, when $n_i \ll (m_1\Delta_1)^{3/2}$, the superexchange at an average distance between impurities is suppressed, and the RKKY interaction gives rise to ferromagnetism, as in the ordinary *pd* model. Corrections due to superexchange can then be calculated using the virial expansion approach.[42] We can rewrite the dominant exchange contribution from Eq. (39) in the following form:

$$J(R) = -J_{\mathrm{RKKY}}F(2p_FR) - V_0\frac{R_0}{R}e^{-R/R_0}, \qquad (61)$$

where $V_0 = \pi J_{\mathrm{RKKY}}/(64p_F^4R_0^4)$, $R_0 = 1/\sqrt{8m_1\Delta_1}$, in case when it is given by one empty band only. If contributions from more than one "empty" band are important, V_0 and J_{RKKY} are, in general, unrelated to each other. The reason for this is that the largest short-range contribution typically comes from the lightest bands, which would produce the longest-range indirect exchange (if all hybridization parameters are of the same order). On the other hand, the dominant RKKY contribution is the one from the heaviest band, since the carriers in that band have the largest Fermi wave vector; there will also be additional RKKY contributions from many bands, which were analyzed in the previous section. In what follows we consider the simplest case, when only one heavy band is relevant for RKKY.

In case of a FS with a direct band gap, the Bloembergen-Rowland mechanism gives rise to ferromagnetism, and we can either have a ferromagnetic or an antiferromagnetic short-range exchange contribution, depending on the relative strength of corresponding exchange processes. If the Boembergen-Rowland term dominates the physics at short distances, the impurity spin Hamiltonian becomes

$$J(R) = -J_{\mathrm{RKKY}}F(2p_FR) + V_{\mathrm{BR}}\frac{R_1}{R}e^{-R/R_1}. \qquad (62)$$

In general, the Bloembergen-Rowland term (40) also has an antiferromagnetic contribution from doped carriers. It then can be rewritten in the following form:

$$J_{12}(R) = V_{\mathrm{BR}}\frac{R_1}{R}e^{-R/R_1} - V_{\mathrm{dop}}\frac{R_g}{R_0}e^{-R/R_g}, \qquad (63)$$

where $R_g = 1/\sqrt{8m_2\Delta_0}$ and V_{BR} and V_{dop} are given by the coefficients in front of exponents in Eqs. (42) and (47). However, since

$$V_{\mathrm{dop}}/V_{\mathrm{BR}} \sim \frac{p_F^3}{(m_1\Delta_1)^{3/2}} \ll 1, \qquad (64)$$

while R_g is still quite small, the contribution of doped carriers to T_c through the Bloembergen-Rowland mechanism can be neglected. Thus, if one exchange process dominates the physics are short distances, the short-range exchange contribution has the same form, and can only differ in sign. In what follows, we consider the general form of exchange integral (61), assuming that the exchange constant V_0, its sign, and its range R_0 are those of the dominant indirect exchange contribution. Note again that in our definition of exchange integral we sum over impurities twice. We will also consider the case when the short-range part in Eq. (61) is rapidly oscillating,

$$J_{\mathrm{SR}} = -V_0\frac{R_0}{R}e^{-R/R_0}\cos(\mathbf{Q}\cdot\mathbf{R}). \qquad (65)$$

As we have seen above, this happens when two bands separated by wave vector $\mathbf{Q}$ contribute the most to the short-range exchange interaction. V_0 has a negative sign for the Bloembergen-Rowland contribution, and a positive sign for the superexchange. When more than one process is important for short-range physics, the problem can always be solved numerically for a given set of parameters. Here we obtain an analytical solution in several limiting cases.

(1) Dilute system with almost no carriers. In the absence of carriers, the type of order and T_c is determined by the short-range part of interaction. If ferromagnetic Bloembergen-Rowland interaction dominates at short distances, Curie temperature is approximately given by the ferromagnetic interaction taken at the average distance between impurities:[6]

$$T_c \simeq 2.3V_0S^2R_0n_i^{1/3}e^{-0.87/R_0n_i^{1/3}}V_0 > 0, \qquad (66)$$

which is valid when $n_i \ll 1/R_0^3$. A comparison with Eq. (3) shows that this gives the following condition on the number of carriers:

$$p_F = (3\pi^3n_e)^{1/3} \ll p_{0F}, \qquad (67)$$

$$p_{0F} = \frac{27.6 V_0 \pi^2 S R_0}{(J^{pd}_{\mathbf{q}=0})^2 (S+1) m^* n_i^{2/3}} e^{-0.87/(R_0 n_i^{1/3})}.$$

When the short-range interaction is antiferromagnetic, it favors spin glass order, and ferromagnetism is absent when there are no or almost no carriers. The condition on the number of carriers for ferromagnetism to be absent is then given by

$$p_F \ll p_{0\mathrm{SG}} = \frac{27.6 |V_0| \pi^2 R_0}{(J^{pd}_{\mathbf{q}=0})^2 m^* n_i^{2/3}} e^{-0.87/(R_0 n_i^{1/3})}. \qquad (68)$$

Finally, for a rapidly oscillating short-range part (65) this condition can be rewritten as

$$p_F \ll p_{0\mathrm{SG}} = \frac{27.6 |V_0| \pi^2 R_0}{(S+1)(J^{pd}_{\mathbf{q}=0})^2 m^* n_i^{2/3}} e^{-0.87/(R_0 n_i^{1/3})}. \qquad (69)$$

For the Anderson Hamiltonian, $J^{pd}_{q=0} = 2V_1^2 a^3/\Delta_1$. Note that if the ratio n_e/n_i is fixed, p_F grows much slower with n_i than p_0. Thus, conditions in Eqs. (67)–(69) are likely to be satisfied at some finite concentration of magnetic impurities $n_c \ll n_i \ll 1/R_0^3$. For example, for antiferromagnetic or oscillating interactions, Eqs. (68) and (69), will define the concentation of impurities above which carrier-driven ferromagnetism disappears.

(2) Dilute system with carriers. When the carrier concentration is large, i.e., $p_F \gg p_0$ in Eqs. (67)–(69), but the concentration of magnetic impurities is still small, $n_i \ll 1/R_0^3$, short-range interactions between magnetic impurities will result in a correction to T_c, which can be calculated by virial expansion (see, for example, Ref. 42). Following Ref. 5, since the range of RKKY interaction is large, we can represent p-d interaction between carriers and magnetic impurities by a mean field Zener Hamiltonian

$$\hat{H}_{\mathrm{MF}} = -J^{pd}_{\mathbf{q}=0} \mathbf{s} \sum_i \mathbf{S}_i, \qquad (70)$$

where **s** is the density of ordered spin of the carriers, which is assumed to be constant in space. In addition, there is a relatively short-range exchange interaction between impurity spins, given by the processes described in Secs. IV and V:

$$\hat{H}_{\mathrm{exch}} = -\sum_{ij} J(\mathbf{R}_i - \mathbf{R}_j) \mathbf{S}_i \cdot \mathbf{S}_j. \qquad (71)$$

The short-range exchange integral does not include the carrier contribution, since it is already accounted for in the mean field Hamiltonian. In the Zener model (70), Curie temperature Eq. (3) can be found by minimizing the free energy density of the system of carriers and spins[5]

$$F = F_e + F_i, \qquad (72)$$

with respect to **s**, and finding when the solution at small s first appears. Here

$$F_e = \frac{(2\mu_B s)^2}{2\chi_0}, \qquad (73)$$

and F_i is given by the usual Zeeman term

$$F_i = -n_i T \ln \frac{\sinh[J^{pd}_{\mathbf{q}=0} s(S+1/2)/T]}{\sinh[J^{pd}_{\mathbf{q}=0} s/(2T)]}. \qquad (74)$$

To find the virial correction to Eq. (3) from Eq. (71), we need to include into F the contribution from two magnetic impurities, when they are close enough:

$$F_{2i} = \frac{1}{2} n_i^2 \int d^3\mathbf{R} [F_{2i}(\mathbf{R}) - 2F_i(\mathbf{R})], \qquad (75)$$

and calculate it from the Hamiltonian

$$\hat{H} = \hat{H}_{\mathrm{MF}} + \hat{H}_{\mathrm{exch}}. \qquad (76)$$

This can be done, since the Zeeman Hamiltonian for two spins, interacting via direct exchange interaction, can easily be solved. The integral over this solution, however, can only be taken with logarithmic accuracy. The contribution from two impurities is important when the distance between them is

$$R \leqslant R_0 \ln \frac{|V_0|/T}{\ln(|V_0|/T)}. \qquad (77)$$

Finding F_{2i}, and repeating the minimization over s, we obtain, as expected, that a for ferromagnetic exchange interaction ($V_0 > 0$) Curie temperature is enhanced:

$$\frac{\delta T_c[F]}{T_c} \simeq \frac{4\pi S}{3(S+1)} n_i R_0^3 \ln^3 \frac{|V_0|/T_c}{\ln(|V_0|/T_c)}. \qquad (78)$$

For an antiferromagnetic exchange interaction ($V_0 < 0$), the Curie temperature is reduced

$$\frac{\delta T_c[A]}{T_c} \simeq -\frac{4\pi}{3} n_i R_0^3 \ln^3 \frac{|V_0|/T_c}{\ln(|V_0|/T_c)}. \qquad (79)$$

A rapidly oscillating exchange interaction (65) gives

$$\frac{\delta T_c[O]}{T_c} \simeq -\frac{4\pi}{3(S+1)} n_i R_0^3 \ln^3 \frac{|V_0|/T_c}{\ln(|V_0|/T_c)}, \qquad (80)$$

which is independent of the sign of V_0.

(3) "Dense" system. The most interesting situation is the case of a "dense" system of magnetic impurities, when $n_i \gg (m_1 \Delta_1)^{3/2}$. Since the short-range part of the interaction could have a range much larger than the lattice spacing, it need not be really dense. This requirement can be rewritten as $n_i \gg (\Delta_1/D)^{3/2}$. In a dense system, the wave functions of the neighboring impurities overlap strongly, and the main exchange contribution arises as a result of this overlap, not the RKKY interaction through free carriers. Then ferromagnetism arises even when no carriers are present, if the Bloembergen-Rowland exchange process dominates the physics at short distances ($V_0 > 0$):

$$T_c = \frac{2S(S+1)n_i}{3} J_{\mathbf{q}=0} = \frac{8\pi S(S+1)n_i}{3} V_0 R_0^3. \qquad (81)$$

Note that T_c does not depend on the carrier concentration, and should be much higher than that resulting from the RKKY interaction.

The Bloembergen-Rowland exchange integral may be weaker than superexchange. In that case, ferromagnetism in a "dense" system is suppressed, and spin glass order is favored. This is always the case for indirect band gap semiconductors, where the short-range ferromagnetic exchange is absent. The Bloembergen-Rowland mechanism in case of direct band gap necessarily leads to an increase of maximum T_c as a function of concentration of magnetic impurities n_i.

VII. APPLICATION TO GAAS:MN

Application of the Anderson model to a real system, such as $Ga_{1-x}Mn_xAs$ is somewhat more involved than the model that we considered above, since Mn ion is in $3d^5$ configuration with a spin $S=5/2$. This configuration has five d orbitals. For symmetry reasons, there may be more than just one conduction or valence band, which is the case for GaMnAs. Then, as we discussed above in Sec. V, one has to take into account all pairwise contributions to the exchange integral, (29) and (30). In particular, there may be unusual contributions to RKKY, such as those considered in Sec. V. In general, one has also to sum over all orbitals in the Anderson Hamiltonian, not just spins, and take the Hund's rule, spin orbit, and crystal field splitting into account. Different orbitals may have different Vs with conduction and valence bands. The result of this treatment, however, produces the same exchange integrals $J(R)$; for example, in case when spin-orbit and crystal field splitting is neglected, the result will still be given by the exchange integral Eqs. (29) and (30), with $|V_1|^2$ is replaced by $\sum_m |V_{1m}|^2$, and similarly for $|V_2|^2$, where V_{1m} is V_1 for mth orbital. The relation between corrections to energy levels and exchange integrals is different in this more realistic case. However, the integrals involved are the same, and, as we have seen above in Sec. III, corrections to energy levels are rather small. Taking Hund's rule into account results in replacing $S=1/2$ operator in equations of the previous section by $\mathbf{S}/(2S)$, with $S=5/2$. Thus, this leads to the same results as in the previous section, with somewhat redefined V's. The relationship between the energy shift and J_{pd} will change, but the actual form of $J(R)$ is determined by the energy spectrum only. Instead of $V_{\alpha m}$, we may introduce

$$|V_\alpha|^2 \equiv \frac{\sum_m |V_{\alpha m}|^2}{4S^2}, \tag{82}$$

and use the form of exchange integrals that we have obtained in the previous sections (with $S=5/2$). Equivalently, this would mean that the expression for $J(\mathbf{R})$ in terms of J_{pd}'s (or J_{RKKY}) for conduction and valence bands and level position will stay the same as in the previous sections.

For a p-type semiconductor, such as $Ga_{1-x}Mn_xAs$, we can adopt an inverted picture, where the "empty" band is now the valence band (empty of holes), while the filled band is the conduction band. The Anderson Hamiltonian is then easily rewritten in terms of holes. There are two types of holes in GaAs—the heavy hole and the light hole. Since their masses are very different ($0.081m_e$ and $0.51m_e$), the main RKKY exchange contribution is produced by the heavy hole. On the other hand, the superexchange contribution from the light hole band has a much larger range, and thus could potentially be more important than the superexchange contribution from the heavy hole band, or the mixed superexchange contribution. However, as we have seen in previous sections, most short range contributions for a direct band gap semiconductor take the form of the second term in Eq. (61), although there may be some variations. The problem is that the amplitude of superexchange $V_0 \propto V^4/D^3 \propto m^3$, where D is the band width. So, for light bands the effective range of the interaction is large, but the payback is that the amplitude turns out to be small. An easy estimate for the light hole band in GaAs shows that for V's of the order of 1 eV this band plays no role in ferromagnetism. The hole mass in the split-off band is $0.15m_e$. This band could also play an important role in the superexchange interaction, although, once again, the amplitude for realistic parameters turns out to be extremely small. The electron mass is $m_{ge}=0.063m_e$ for the main Γ valley. The masses and gaps for L and X valleys are much larger, so we do not expect them to play much role. Thus, we arrive at a simplified picture, where only the heavy hole band and Γ-valley electrons are relevant. The CFR Mn d^6/d^5 level, which is important for our analysis, is in the conduction band, $\Delta_1=1.5$ eV above the top of the valence band. We can see from Eqs. (45) and (35) that, for this particular level position, the ferromagnetic Bloembergen-Rowland interaction has the range $R_0 \equiv R_{\mathrm{BR}} \simeq \hbar/\sqrt{2m_{hh}\Delta_1}$, while the range of the superexchange is $R_{se} \simeq R_{\mathrm{BR}}/2$. The amplitude of the Bloembergen-Rowland term $V_{\mathrm{BR}}/V_{se} \simeq V_2^2 m_{ge}/(2V_1^2 m_{hh})$, could become comparable or exceed the amplitude of heavy hole superexchange. Note that, in case of strong short-range ferromagnetic interaction, it would be energetically favorable for Mn impurities to form ferromagnetic clusters. This, in turn, would reduce the Curie temperature. Clustering of Mn impurities would make magnetic properties of this material crucially dependent on sample preparation. On the other hand, antiferromagnetic short-range interactions should be stronger at shorter distances, which would potentially lead to an exchange integral (in the absence of carriers), which changes its sign as a function of the distance between impurities. In general, for the particular situation when the Mn level is almost at the bottom of conduction band, the range of antiferromagnetic superexchange is approximately $R_0/2$, and we may represent the total short-range exchange integral in the following form:

$$J(R) \simeq V_0 \frac{R_0}{R}[-\alpha \exp(-2R/R_0) + \exp(-R/R_0)]. \tag{83}$$

Here $V_0=V_{\mathrm{BR}}>0$, while $\alpha \simeq m_{hh}V_1^2/(m_{ge}V_2^2)$ is the ratio of superexchange and Bloembergen-Rowland amplitudes (up to a factor of 2), which depends on the hybridization of impurity d level with the valence band (V_2), of impurity d level with the heavy hole band V_{hh} and the corresponding effective masses. When $\alpha>1$ (which is likely the case here, since $m_{hh} \gg m_{ge}$), the exchange becomes antiferromagnetic at short distances for $R<R_0 \ln \alpha$. The virial correction to T_c for such exchange integral (assuming T_c is determined mostly by the

p-d interaction of magnetic impurities and heavy holes) is then given by

$$\frac{\delta T_c}{T_c} \simeq \frac{4\pi S}{3(S+1)} n_i R_0^3 \left(\ln^3 \frac{V_0/T_c}{\ln(V_0/T_c)} - [2+(1/S)]\ln^3 \alpha \right), \tag{84}$$

and could change sign as well, at some large doping level. If carriers are not present, this exchange integral alone, for $\alpha > 1$, would lead to a saturation or decrease of T_c at large doping. On the other hand, when $\alpha < 1$, ferromagnetism gets significantly enhanced at short distances.

In general, the interplay between various short range contributions leads to a rather complicated physics at short distances. While a detailed calculation requires precise knowledge of all hybridization parameters from the quantum chemistry, we can estimate the Mn concentration at which the short distance physics becomes important by requiring $\delta T_c / T_c \sim 0.5$ in Eq. (84). We take the estimate of $J_{pd} \sim 150$ eV Å^3 and $T_c \sim 110$ K from Ref. 13, $\Delta_1 \sim 1.5$ eV, and assume that $\alpha \simeq 1$. Then $V_0 = J_{pd}^2 m_{hh}^3/(8\pi^2)$, and we get

$$x_i \sim \left(\frac{a}{2R_0 \ln(V_0/T_c)} \right)^3 \sim 8\,\% . \tag{85}$$

Finally, it should be mentioned that there is another ferromagnetic contribution to shorter-range exchange, coming from the Anderson model and Hunds rule ferromagnetic exchange for realistic systems. This ferromagnetic exchange corresponds to the following process: a Mn *d* hole is taken into the *s-p* hole band at another Mn site, followed by the Hunds-rule ferromagnetic exchange on another Mn. Only one hole band participates in this virtual process. This gives the ferromagnetic contribution of the form[28]

$$J_{\mathrm{HF}}(R) = -\frac{V_1^2 a^3 J_H m_1^2}{4\pi^2 R^2} e^{-2\sqrt{2m_1\Delta_1}R}, \tag{86}$$

which shows that the direct band gap is not necessary for ferromagnetism at shorter distances, and for the physics discussed above. A different power of R would introduce minor corrections in the results discussed above, such as the change the power of concentration in Eq. (66) from $n_i^{1/3}$ to $n^{2/3}$, and R in Eq. (77) to

$$R \leqslant R_0 \ln \frac{|V_0|/T}{\ln^2(|V_0|/T)}. \tag{87}$$

Finally, it should be mentioned that percolation can only be treated analytically in some limiting cases. Detailed Monte Carlo calculations, such as the simulations done in Ref. 43 are absolutely crucial for understanding the problem.

VIII. EFFECTS OF DISORDER AND INTERACTIONS

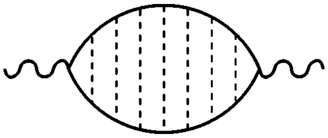

FIG. 8. Impurity corrections to Curie temperature.

In this section we consider rather briefly effects of disorder and interactions. Since the superexchange and the Bloembergen-Rowland exchange interaction are governed by high-energy virtual processes, they are independent of disorder. The RKKY interaction, however, gets modified. This modification was first considered by de Gennes,[44] who argued that, since the RKKY interaction at large distances is dominated by the $2p_F$ Kohn anomaly wave vector, the vertex corrections are not essential for the averages over disorder. The long-distance power law in the RKKY interaction then gets multiplied by an exponential factor $\exp(-2R/l)$, where l is the scattering length. These effects were indeed taken into account by Ohno *et al.*[13] in their original paper. Abrahams *et al.*,[45] however, have shown that this is not the whole story, since disorder introduces instead a *distribution* of $J(R)$ at large distances. We note here that the long-distance behavior of the RKKY interaction is not essential for ferromagnetism. The Curie temperature is determined by RKKY exchange at short distances, or $J_{\mathrm{RKKY}}(\mathbf{q}=0)$. Of course, the vertex corrections are essential for the calculation of the RKKY loop diagram at $\mathbf{q}=0$. Summing all ladder diagrams (0 order in $1/p_F l$), shown in Fig. 8, leads to a diffuson contribution

$$\Pi(\mathbf{q},\omega_n) = -\frac{\nu D \mathbf{q}^2}{|\omega_n| + D\mathbf{q}^2}, \tag{88}$$

which significantly modifies frequency dependence of RKKY at $\mathbf{q}=0$. Here D is the diffusion coefficient.

However, the static ($\omega=0$), not dynamic, part of the diagram in Fig. 8 determines T_c, and it is not changed at all. Thus, to the leading order in $1/p_F l$ disorder does not modify the Curie temperature. The interactions, if not too strong, can also be included as the standard Fermi-liquid corrections to χ_0 in Eq. (3). Weak localization corrections (the Cooperon diagrams), however, should modify T_c. They can also be included in the same way as the standard weak localization corrections to spin susceptibility (see, for example, Ref. 46), and Eq. (3) should still be valid.

Finally, we note that strong exchange interaction J^{pd} could bind holes at Mn sites, forming a shallow (or deep) complex magnetic impurity. This effect would reduce the hole concentration and the number of free Mn spins, and thus lead to a reduction Curie temperature. The interactions between these complex magnetic impurities would be determined by the overlap of the corresponding wave functions.

IX. CONCLUSIONS

We have investigated the model of magnetic semiconductors in which magnetic impurities are treated in the framework of the Anderson model. We have shown that the effective Hamiltonian of this model is more rich than the usual *p-d* model considered in the literature. Effectively, in the Anderson model, wave functions of localized impurities develop a “tail,” which could be long range. When the concentration of magnetic impurities is large enough, the overlap of wave functions on two different sites leads to a very strong exchange interaction, which is important, and could dominate the physics at Mn concentrations as low as 5%. There are two contributions to this exchange interaction-superexchange, in which localized electrons are exchanged trough only one type of bands (either conduction or valence bands), and the Bloumbergen-Rowland term, when the exchange is through both conduction and valence bands. We have found that, in case of direct band gap, the Bloemberger-Rowland exchange is ferromagnetic. This could lead to a dramatic enhancement of Curie temperatures in certain magnetic semiconductors with a direct band gap, such as GaMnAs. One other important consequence of the indirect exchange is that, if it is ferromagnetic and reasonably long range, doped carriers are not necessary to mediate ferromagnetism. This leads potentially to a new class of high-temperature magnetic semiconductors, with high Curie temperatures determined entirely by the interaction between localized impurities, *not Zener mechanism*. This emphasizes the effort to search for new materials, where ferromagnetism is not carrier driven (for example, driven by the Bloembergen-Rowland mechanism). Another important consequence of the Anderson model is that, if there are more than one type of carriers (for example, light and heavy holes in GaAs), the long-range RKKY interaction becomes rather complicated, since it involves a "mixed" contribution. We have also found that, at large doping, the RKKY interaction for the Anderson model and the *p-d* model is *different* at short distances. The effective exchange interaction in the $U=\infty$ Anderson model for any FS is given by Eqs. (19), (29), and (30). A numerical solution of this effective Hamiltonian for a given set of parameters (determined from quantum chemistry) would give the answer for $T_c(n_i)$ in the most general case.

We have briefly considered effects of disorder and interactions. We have shown that when De Gennes[44] approximation $p_F l \gg 1$ is applicable, disorder does not modify Curie temperature. Localization effects, however, do modify Curie temperature, although their effect could be reduced to removal carriers. Finally, in this paper we have not considered the effects of mixing of conduction and valence bands (such as *kp*). These effects should also be included in the full description. We should mention that application of the Anderson model to GaAs:Mn was also considered in Ref. 47, although the limits of the Anderson model and their conclusions are different from ours.

ACKNOWLEDGMENTS

I would like to thank L. P. Gor'kov, Z. Fisk, and G. Kotliar for many useful discussions, and H. Weitering for sharing his experimental observations. I am also very greatful to Misha Zhitomirsky for pointing out Ref. 47. This work was supported by the University of Tennessee.

---

[1] G. A. Prinz, Science **282**, 1660 (1998).

[2] S. A. Wolf, D. D. Awschalom, R. A. Buhrman, J. M. Daughton, S. von Molnár, M. L. Roukes, A. Y. Chtchelkanova, and D. M. Treger, Science **294**, 1488 (2001).

[3] C. Zener, Phys. Rev. **81**, 440 (1951).

[4] C. Zener, Phys. Rev. **83**, 299 (1951).

[5] A. A. Abrikosov and L. P. Gor'kov, Zh. Eksp. Teor. Fiz. **43**, 2230 (1962).

[6] I. Ya. Korenblit and E. F. Shender, Usp. Fiz. Nauk **126**, 233 (1978) [Sov. Phys. Usp. **21**(10), 832 (1978)].

[7] J. K. Furdyna and J. Kossut, *Diluted Magnetic Semiconductors*, vol. 25 of *Semiconductor and Semimetals* (Academic Press, New York, 1988).

[8] T. Dietl, *Diluted Magnetic Semiconductors*, vol. 3B of *Handbook of Semiconductors* (North-Holland, New York, 1994).

[9] T. Dietl, H. Ohno, F. Matsukura, J. Cibert, and D. Ferrand, Science **287**, 1019 (2000).

[10] T. Dietl, H. Ohno, and F. Matsukura, Phys. Rev. B **63**, 195205 (2001).

[11] H. Munekata, H. Ohno, S. von Molnar, A. Segmüller, L. L. Chang, and L. Esaki, Phys. Rev. Lett. **63**, 1849 (1989).

[12] J. De Boeck, R. Oesterholt, A. Van Esch, H. Bender, C. Bruynseraede, C. Van Hoof, and G. Borghs, Appl. Phys. Lett. **68**, 2744 (1996).

[13] F. Matsukura, H. Ohno, A. Shen, and Y. Sugawara, Phys. Rev. B **57**, R2037 (1998).

[14] H. Ohno, A. Shen, F. Matsukura, A. Oiwa, A. Endo, S. Katsumoto, and Y. Iye, Appl. Phys. Lett. **69**, 363 (1996).

[15] H. Ohno, Science **281**, 951 (1998).

[16] Y. D. Park, A. T. Hanbicki, S. C. Erwin, C. S. Hellberg, J. M. Sullivan, J. E. Mattson, T. F. Ambrose, A. Wilson, G. Spanos, and B. T. Jonker, Science **295**, 651 (2002).

[17] K. C. Ku *et al.*, Appl. Phys. Lett. **82**, 2302 (2003).

[18] K. W. Edmonds *et al.*, Phys. Rev. Lett. **92**, 037201 (2004).

[19] A. Chattopadhyay, S. Das Sarma, A. J. Millis, Phys. Rev. Lett. **87**, 227202 (2001).

[20] M. J. Calderon, G. Gomez-Santos, and L. Brey, Phys. Rev. B **66**, 075218 (2002).

[21] M. Auslender and E. Kogan, Phys. Rev. B **65**, 012408 (2001).

[22] T. Jungwirth, J. König, J. Sinova, J. Kucera, and A. H. MacDonald, Phys. Rev. B **66**, 012402 (2002).

[23] L. Brey and G. Gomez-Santos, Phys. Rev. B **68**, 115206 (2003).

[24] J. Schliemann and A. H. MacDonald, Phys. Rev. Lett. **88**, 137201 (2002); J. Schliemann, Phys. Rev. B **67**, 045202 (2003).

[25] G. Zaránd and B. Janko, Phys. Rev. Lett. **89**, 047201 (2002).

[26] A. Kaminski and S. Das Sarma, Phys. Rev. Lett. **88**, 247202 (2002).

[27] A. Kaminski and S. Das Sarma, Phys. Rev. B **68**, 235210 (2003).

[28] D. I. Khomskii and D. A. Sawatzky, Solid State Commun. **102**, 87 (1997).

[29] V. G. Vaks, A. I. Larkin, S. A. Pikin, Zh. Eksp. Teor. Fiz. **53**, 281 (1967); **53**, 1089 (1967).

[30] D. P. Young, D. Hall, M. E. Torelli, Z. Fisk, J. L. Sarrao, J. D. Thompson, H. R. Ott, S. B. Oseroff, R. G. Goodrich, and R. Zysler, Nature (London) **397**, 412 (1999).

[31] J. Akimitsu, K. Takenawa, K. Suzuki, H. Harima, and Y. Kura-

moto, Science **293**, 1125 (2001).

[32] Z. Fisk, H. R. Ott, V. Barzykin, and L. P. Gor'kov, Physica B **312–313**, 808 (2002).

[33] K. Matsubayashi, M. Maki, T. Tsuzuki, T. Nishioka, and N. K. Sato, Nature (London) **420**, 143 (2002).

[34] J. R. Schrieffer and P. A. Wolff, Phys. Rev. **149**, 491 (1966).

[35] L. P. Gor'kov, A. V. Sokol, J. Phys. (France) **50**, 2823 (1989); L. P. Gor'kov and A. V. Sokol, Pis'ma Zh. Eksp. Teor. Fiz. **48**, 505 (1988).

[36] V. Barzykin and L. P. Gor'kov, Phys. Rev. B **46**, 3059 (1992).

[37] N. Bloembergen and T. J. Rowland, Phys. Rev. **97**, 1679 (1955).

[38] L. P. Gor'kov and A. V. Sokol, Physica C **159**, 329 (1989).

[39] B. E. Larson, K. C. Hass, H. Ehrenreich, and A. E. Carlsson, Phys. Rev. B **37**, 4137 (1988).

[40] L. V. Keldysh, Zh. Eksp. Teor. Fiz. **45**, 364 (1963).

[41] A. A. Abrikosov, Adv. Phys. **29**, 869 (1980).

[42] V. Barzykin and I. Affleck, Phys. Rev. B **61**, 6170 (2000).

[43] J. Schliemann, J. König, H.-H. Lin, and A. H. MacDonald, Appl. Phys. Lett. **78**, 1550 (2001); J. Schliemann, J. König, and A. H. MacDonald, Phys. Rev. B **64**, 165201 (2001).

[44] P. J. de Gennes, J. Phys. Radium **23**, 630 (1962).

[45] A. Jagannathan, E. Abrahams, and M. J. Stephen, Phys. Rev. B **37**, 436 (1988).

[46] P. A. Lee, T. V. Ramakrishnan, Rev. Mod. Phys. **57**, 287 (1985).

[47] P. M. Krstajić, V. A. Ivanov, F. M. Peeters, V. Fleurov, and K. Kikoin, Europhys. Lett. **61**, 235 (2003).