RKKY interaction in semiconductors: Effects of magnetic field and screening

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We derive the Ruderman-Kittel-Kasuya-Yosida (RKKY) theory for semiconductors including band degeneracy, modulation of the band edges, and external fields. Explicit expressions are given for a three- and two-dimensional semiconductor in a magnetic field. Screening effects are included by calculating the density correlation function. We show that the RKKY theory with screening is equivalent to the mean-field Zener model.

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I. INTRODUCTION

Diluted magnetic semiconductors (DMS) have been extensively studied for more than a decade.[1,2] The exchange coupling between magnetic ions and electrons leads to a giant effective *g* factor. In recent years, ferromagnetism in Mn-doped III-V and II-VI semiconductors has been predicted theoretically[3–7] and measured experimentally;[8–14] for a review, see Ref. 15. In low-dimensional semiconductors, ferromagnetism can be controlled through the modulation of the band edges, external fields, and carrier injection by optical pulses.[7,12,14] The goal is the development of semiconductor devices which use the spin degree of freedom for the storage and processing of information, known as spintronics.[16,17]

The indirect exchange interaction of magnetic ions by electrons has been explained by the Ruderman-Kittel-Kasuya-Yosida (RKKY) theory, developed in the 1950s,[18–20] and by a mean-field Zener theory, which goes back to papers by Stoner from the 1930s.[21] The range function of the RKKY interaction has been calculated already in the early papers for interaction-free electrons in three, two, and one dimension, both in momentum[22] and in real space.[22–25] Dietl *et al.*,[3] assuming only the lowest subband to be occupied, expressed the RKKY interaction of a low-dimensional semiconductor in terms of the range function of the ideal three-, two-, and one-dimensional electron gas.

However, realistic low-dimensional semiconductors are never perfectly two or one dimensional. For example, quantum wells and superlattices have an effective dimension between two and three, quantum wires between one and two. As the translational symmetry is broken in the directions of confinement, the range function does no longer depend only on the difference of the coordinates. It is quite common to treat Bloch electrons like free electrons and few papers pay attention to the details of the band structure.[4,26–28]

Moreover, the magnetic field itself leads to a quantization of the electron and hole motion and to reduction of the dimensionality. For example, a bulk semiconductor in a magnetic field has features both of a three- and of a one-dimensional semiconductor. To describe experiments in high magnetic fields, it is no longer justified to assume the RKKY interaction to be the same as in the field-free case and the influence of the magnetic field on the range function needs to be taken into account.

An open problem is the effect of screening. It was argued on the basis of the diagram technique that screening plays no role in the absence of Zeeman splitting.[29] In semiconductors, Zeeman splitting is usually not negligible. The spin susceptibility, including screening, was calculated already in the late sixties,[30] but these results did not make their way into the theory of ferromagnetism in semiconductors. It is also not clear if the perturbation-theoretical character of the RKKY theory limits its validity and in which way RKKY theory and mean-field Zener theory are related to each other.

In this paper, we present a rigorous derivation of the RKKY theory for semiconductors. First, in Sec. II, we derive the RKKY interaction by means of both perturbation theory and Kubo theory and show the equivalence. Then, in Sec. III, we derive the effective RKKY Hamiltonian for low-dimensional semiconductors, including the sample geometry, band degeneracy, and external fields. To illustrate the usefulness of the theory, in Sec. IV we derive analytical results for a bulk semiconductor and an ideally two-dimensional semiconductor in a magnetic field. The results are compared with the range functions for the three-, two-, and one-dimensional electron gas, and limiting cases are studied. In Sec. V, we calculate the range function in the presence of screening and show the equivalence of RKKY theory including screening and mean-field Zener theory. Summary and conclusions are given in Sec. VI.

II. THE RKKY INTERACTION

The derivation of the effective Hamiltonian by second-order perturbation theory in the original paper by Ruderman and Kittel is somewhat hand waving.[18] An alternative approach to the effective interaction is based upon the magnetic susceptibility, which was pioneered by Wolff.[29,31] Here we give a rigorous derivation of the effective Hamiltonian by Löwdin's perturbation theory and by linear response theory, which gives the same result. The effective interaction is related to the density correlation function, which allows us to systematically study the role of many-particle effects.

A. Degenerate perturbation theory

We start with Löwdin's degenerate perturbation theory. Suppose the Hamiltonian of a system is of the form

$$H = \begin{pmatrix} H_{AA} & H_{AB} \\ H_{BA} & H_{BB} \end{pmatrix}. \tag{1}$$

The block indices correspond to Löwdin's classes A and B for the resonant and off-resonant eigenstates. The elements of the diagonal blocks are $H_{AAjj'}=E_j\delta_{jj'}$ for $j,j'\in A$ and $H_{BBjj'}=E_j\delta_{jj'}$ for $j,j'\in B$. The nondiagonal blocks, which contain the perturbation, may be fully occupied and fulfill $H_{BA}=H_{AB}^{\dagger}$. Then, in second-order perturbation theory, the eigenvalue problem of the class A solutions is determined by an effective Hamiltonian[32]

$$H_{\mathrm{eff}\,jj'} = E_j\delta_{jj'} + \sum_{j''\in B} \frac{H_{jj''}H_{j''j'}}{E_j - E_{j''}}, \quad j,j'\in A. \tag{2}$$

We assume that N magnetic ions with magnetic moments $\hat{\mathbf{S}}_1,\ldots,\hat{\mathbf{S}}_N$ with g (or Landé) factor g_{ion} are located at the lattice points $\mathbf{R}_1,\ldots,\mathbf{R}_N$. The magnetic ions are equally distributed so that the material is macroscopically homogeneous. The probability of a lattice site being occupied by a magnetic ion is equal to the mole fraction $x\in[0,1]$. (For semiconductors with two cations per unit cell, in the resulting expressions, x has to be replaced by $2x$.)

As the direct interaction between their angular momenta is negligible, the unperturbed Hamiltonian of the ions $\hat{H}_{\mathrm{ion}}$ is a constant. The orthonormal and complete eigenstates of the ionic system are given by

$$|M_1,\ldots,M_N\rangle = |S,M_1\rangle\otimes\cdots\otimes|S,M_N\rangle,$$

where S is the quantum number of the total angular momentum of a magnetic ion, which is the same for all ions, and $M_j\in\{+S,\ldots,-S\}$ is the projection of the jth angular momentum (here, onto the z axis). The dimension of the eigenspace for the ionic system is $(2S+1)^N$.

The eigenstates and eigenenergies of the subsystem of P electrons are given by $|\Gamma\rangle$ and $\mathcal{E}_\Gamma$, where Γ_0 denotes the ground state. The exchange interaction between electrons and magnetic ions is

$$\hat{H}_{\mathrm{el\text{-}ion}} = \sum_{k=1}^{P}\sum_{j=1}^{N} \hat{\mathbf{S}}_j\cdot\mathbf{s}_k I(\mathbf{r}_k-\mathbf{R}_j) = \sum_{j=1}^{N}\int d^3\mathbf{r}\hat{\mathbf{S}}_j\cdot\hat{\mathbf{s}}(\mathbf{r})I(\mathbf{r}-\mathbf{R}_j), \tag{3}$$

where I is a real, strongly localized function and $\mathbf{s}=\hbar/2(\sigma_x,\sigma_y,\sigma_z)^T$ is the electron spin operator with eigenstates $|s=\frac{1}{2},m=\pm\frac{1}{2}\rangle=|s=\frac{1}{2},m=\uparrow,\downarrow\rangle$. In second quantization, the operator of the spin density is expressed in terms of field operators as

$$\hat{\mathbf{s}}(\mathbf{r}) = \sum_{mm'} \hat{\psi}_m^{\dagger}(\mathbf{r})\mathbf{s}_{mm'}\hat{\psi}_{m'}(\mathbf{r}). \tag{4}$$

The interaction (3) has the same structure, like a spin orbit or hyperfine interaction.

After these preparations, we are able to identify the components of the Hamiltonian (1). The ground state of the interaction-free electron-ion system, which is identified with Löwdin's class A, is given by $|\Gamma_0\rangle\otimes|M_1,\ldots,M_N\rangle$. Without loss of generality, its energy is set equal to zero. The multiplicity of the ground state is $(2S+1)^N$. Therefore, H_{AA} in Eq. (1) is a square matrix of dimension $(2S+1)^N$, with all elements being zeros. Likewise, the excited states are $|\Gamma\rangle\otimes|M_1,\ldots,M_N\rangle$, where $\Gamma\neq\Gamma_0$. Their multiplicity is also $(2S+1)^N$. Consequently, H_{BB} is a diagonal matrix with elements $\mathcal{E}_\Gamma$; $\Gamma\neq\Gamma_0$, where each $\mathcal{E}_\Gamma$ appears $(2S+1)^N$ times.

The sum in Eq. (2) has to be carried out over all excited electron states Γ and over all angular-momentum quantum numbers $M_1,\ldots,M_N$ of the magnetic ions. As the unperturbed energies of the magnetic ions are independent of the ion spin projections, the sum over the $M_1,\ldots,M_N$ is equivalent to inserting a $(2S+1)^N$-dimensional identity matrix. Furthermore, instead of calculating all $(2S+1)^N\times(2S+1)^N$ matrix elements of H_{eff}, we can directly calculate the effective Hamiltonian, acting in the subspace of the magnetic ions, just by dropping $\langle M_1,\ldots,M_N|$ and $|M_1',\ldots,M_N'\rangle$ on the left and right side, respectively. Then the Hamiltonian of the effective ion-ion interaction becomes

$$\hat{H}_{\mathrm{ion\text{-}ion}} = -\sum_{jj'}\sum_{\Gamma}{}' \frac{1}{\mathcal{E}_\Gamma-\mathcal{E}_{\Gamma_0}} \langle\Gamma_0|\hat{\mathbf{S}}_j\cdot\int d^3\mathbf{r}I(\mathbf{r}-\mathbf{R}_j)\hat{\mathbf{s}}(\mathbf{r})|\Gamma\rangle \times\langle\Gamma|\int d^3\mathbf{r}'I(\mathbf{r}'-\mathbf{R}_{j'})\hat{\mathbf{s}}(\mathbf{r}')\cdot\hat{\mathbf{S}}_{j'}|\Gamma_0\rangle. \tag{5}$$

The prime at the sum means that the ground state Γ_0 is excluded.

We shall now evaluate the expression (5) in a mean-field (e.g., Hartree, Hartree-Fock) approximation, where the many-particle state $|\Gamma\rangle$ is an antisymmetrized tensor product (Slater determinant) of effective single-particle states. We denote the single-electron eigenstates and eigenenergies by $|\gamma\rangle$ and E_γ, where $E_{\gamma'}>E_\gamma$ for $\gamma'>\gamma$. With the introduction of creation and annihilation operators,

$$\hat{\psi}_m^{\dagger} = \sum_{\gamma}\hat{a}_\gamma^{\dagger}\varphi_{\gamma;m}^{*}(\mathbf{r}), \quad \hat{\psi}_m = \sum_{\gamma}\varphi_{\gamma;m}(\mathbf{r})\hat{a}_\gamma,$$

the electron ground state is written as

$$|\Gamma_0\rangle = \hat{a}_P^{\dagger}\cdots\hat{a}_1^{\dagger}|\rangle, \tag{6}$$

where $|\,\rangle$ is the vacuum state, when no electron is present. Only excited states of the form

$$|\Gamma\rangle = \hat{a}_{\gamma'}^{\dagger}\hat{a}_\gamma|\Gamma_0\rangle; \quad \gamma\in\{1,\ldots,P\}, \quad \gamma'\notin\{1,\ldots,P\} \tag{7}$$

contribute to the sum (5) and the resulting effective Hamiltonian is

$$\hat{H}_{\mathrm{ion\text{-}ion}} = -\sum_{jj'}\sum_{\gamma\gamma'}\frac{f_\gamma(1-f_{\gamma'})}{E_{\gamma'}-E_\gamma} \times\hat{\mathbf{S}}_j\cdot\sum_{m_1m_1'}\int d^3\mathbf{r}\varphi_{\gamma;m_1}^{*}(\mathbf{r})\mathbf{s}_{m_1m_1'}I(\mathbf{r}-\mathbf{R}_j)\varphi_{\gamma';m_1'}(\mathbf{r}) \times\sum_{m_2m_2'}\int d^3\mathbf{r}'\varphi_{\gamma';m_2}^{*}(\mathbf{r}') \times\mathbf{s}_{m_2m_2'}I(\mathbf{r}'-\mathbf{R}_{j'})\varphi_{\gamma;m_2'}(\mathbf{r}')\cdot\hat{\mathbf{S}}_{j'}, \tag{8}$$

which is the RKKY Hamiltonian. The occupation numbers f_γ take the values 0 and 1, depending on whether the state $|\gamma\rangle$ is occupied or not. The formulation of the interaction in second quantization (4) is independent of the number of electrons and the derivation remains valid for a statistical ensemble when f_γ is replaced by the Fermi function.

B. Kubo theory

Formally, the RKKY interaction can be derived by means of Kubo theory and the effective Hamiltonian can be expressed in terms of the magnetic susceptibility. The interaction of the electrons with an external magnetic field $\mathbf{H}(\mathbf{r},t)$ is given by

$$\hat{H}^{(\mathrm{i})}(t) = \frac{\mu_0 e}{m_0} \int d^3\mathbf{r}\hat{\mathbf{s}}(\mathbf{r},t)\cdot\mathbf{H}(\mathbf{r},t) \tag{9}$$

and the induced magnetization is

$$\mathbf{M}(\mathbf{r},t) = -\frac{\mu_0 e}{m_0}\langle\hat{\mathbf{s}}(\mathbf{r},t)\rangle.$$

According to Kubo theory,[33,34] the linear response of the electron gas is

$$M_\alpha(\mathbf{r},\omega) = \mu_0 \sum_{\alpha'} \int d^3\mathbf{r}'\chi_{\mathrm{ret}\alpha\alpha'}(\mathbf{r},\mathbf{r}',\omega)H_{\alpha'}(\mathbf{r}',\omega) \tag{10}$$

with the susceptibility

$$\chi_{\mathrm{ret}\alpha\alpha'}(\mathbf{r},\mathbf{r}',\omega) = \frac{1}{\mu_0}\left(\frac{\mu_0 e}{m_0}\right)^2 \frac{i}{\hbar}\int_0^\infty dt\, e^{+i(\omega+i\epsilon)t}\langle[\hat{s}_\alpha(\mathbf{r},t),\hat{s}_{\alpha'}(\mathbf{r}',0)]\rangle, \tag{11}$$

where $\epsilon=+0$ is a positive infinitesimal. For a static magnetic field, the change of the energy caused by the magnetization of the electrons is

$$-\frac{1}{2}\mu_0\sum_{\alpha\alpha'}\int d^3\mathbf{r}\int d^3\mathbf{r}' H_\alpha(\mathbf{r})\chi_{\mathrm{ret}\alpha\alpha'}(\mathbf{r},\mathbf{r}',\omega=0)H_{\alpha'}(\mathbf{r}'). \tag{12}$$

Formally, the interaction with the magnetic field (9) is equal to the electron-ion interaction (3), if we identify

$$\mathbf{H}(\mathbf{r}) = \frac{m_0}{\mu_0 e}\sum_j \hat{\mathbf{S}}_j I(\mathbf{r}-\mathbf{R}_j).$$

(It is worthwhile to note that **H** in this expression has nothing to do with the magnetic field caused by the ions.) Then the energy change (12) can be identified with the effective Hamiltonian

$$\hat{H}_{\text{ion-ion}} = -\frac{1}{2}\mu_0\left(\frac{m_0}{\mu_0 e}\right)^2\sum_{jj'}\sum_{\alpha\alpha'}\int d^3\mathbf{r}\int d^3\mathbf{r}' \times \hat{S}_{j\alpha} I(\mathbf{r}-\mathbf{R}_j)\chi_{\mathrm{ret}\alpha\alpha'}(\mathbf{r},\mathbf{r}',\omega=0)I(\mathbf{r}'-\mathbf{R}_{j'})\hat{S}_{j'\alpha'}. \tag{13}$$

Indeed, the expressions (5) and (13) are identical, except for the contribution at $j=j'$. The reason is that, in contrast to the classical field (12), the ion spin operators do not commute in the general case, more strictly, it holds that $[\hat{S}_{j\alpha},\hat{S}_{j',\alpha+1}]=i\hbar\hat{S}_{j,\alpha+2}\delta_{jj'}$. As we consider only extended systems, the contributions for $j=j'$ are negligible and can be dropped, as usually done in the literature.

In the language of many-particle physics, the magnetic susceptibility is given by

$$\chi_{\mathrm{ret}\alpha\alpha'}(\mathbf{r},\mathbf{r}',\omega) = -\frac{1}{\mu_0}\left(\frac{\mu_0 e}{m_0}\right)^2\sum_{m_1m_1'}\sum_{m_2m_2'} \times s_{\alpha m_1 m_1'}L_{\mathrm{ret}m_1'm_1,m_2'm_2}(\mathbf{r},\mathbf{r}',\omega)s_{\alpha' m_2 m_2'}, \tag{14}$$

where L is the density correlation function.[35,36] This representation is helpful to systematically study the role of the electron-electron interaction, which will be done in Sec. V. It also allows us to consistently include nondiagonal elements of the density matrix, which play a role in coherently excited semiconductors. The approximation of the $|\Gamma\rangle$ by uncorrelated states (6) and (7) is equivalent to the following approximation of the density correlation function:

$$L(\underline{1},\underline{1}',\underline{2},\underline{2}') \approx \Pi^{(0)}(\underline{1},\underline{1}',\underline{2},\underline{2}') = -i\hbar G(\underline{1},\underline{2}')G(\underline{2},\underline{1}'). \tag{15}$$

The evaluation of $\Pi^{(0)}$ is tedious but straightforward,[36] and the result for the effective Hamiltonian is

$$\hat{H}_{\text{ion-ion}} = -\frac{1}{2}\sum_{jj'}\sum_{\gamma\gamma'}\frac{f_\gamma - f_{\gamma'}}{E_{\gamma'}-E_\gamma} \times \hat{\mathbf{S}}_j\cdot\sum_{m_1m_1'}\int d^3\mathbf{r}\varphi^*_{\gamma;m_1}(\mathbf{r})\mathbf{s}_{m_1m_1'}I(\mathbf{r}-\mathbf{R}_j)\varphi_{\gamma';m_1'}(\mathbf{r}) \times \sum_{m_2m_2'}\int d^3\mathbf{r}'\varphi^*_{\gamma';m_2}(\mathbf{r}') \times \mathbf{s}_{m_2m_2'}I(\mathbf{r}'-\mathbf{R}_{j'})\varphi_{\gamma;m_2'}(\mathbf{r}')\cdot\hat{\mathbf{S}}_{j'}. \tag{16}$$

This is the same as expression (8) symmetrized in the variables $\hat{S}_{j\alpha}$ and $\hat{S}_{j'\alpha'}$. Due to the positive infinitesimal ϵ in Eq. (11), the sum over the eigenstates has to be interpreted as Cauchy's principal value.

Suppose that the effective Hamiltonian (16) at zero temperature is known as a function of the Fermi energy E_F. Then, by virtue of the relation

$$\frac{1}{\exp\dfrac{E-\mu}{k_BT}+1} = \int_{-\infty}^{+\infty} dE_F \frac{1}{4k_BT}\,\mathrm{sech}^2\,\frac{\mu-E_F}{2k_BT}\Theta(E_F-E),$$

the effective Hamiltonian as function at finite temperature is given by

$$\hat{H}_{\text{ion-ion}}(T,\mu) = \int_{-\infty}^{+\infty} dE_F \frac{1}{4k_BT} \operatorname{sech}^2 \frac{\mu - E_F}{2k_BT} \hat{H}_{\text{ion-ion}}(T=0,E_F). \tag{17}$$

This equation is valid for any quantity that is a linear functional of the Fermi function. The integral kernel has a width of the order of k_BT and a weight 1. Formula (17) can be generalized to nonequilibrium distributions, as occur in highly excited semiconductors. Then the integral kernel is given by the derivative of the occupation number with respect to the energy.

III. RKKY INTERACTION IN LOW-DIMENSIONAL SEMICONDUCTORS

We shall now derive the RKKY interaction for low-dimensional semiconductors, including band degeneracy and external fields. We start with the general expression and then consider a twofold degenerate band. Explicit expressions are given for the case with and without Zeeman splitting.

A. Envelope-function representation

In a low-dimensional semiconductor, the eigenfunctions can approximately be represented by products of slowly varying functions, so-called envelope functions, and lattice-periodic functions. Let ν be an energy band which is L-fold degenerate at the Γ point ($\mathbf{k}=0$). The lattice-periodic parts of the Bloch functions at $\mathbf{k}=0$ are $u_{\nu,l,\mathbf{k}=0;m}(\mathbf{r}) = u_{\nu l;m}(\mathbf{r})$; $l = 1,\ldots,L$. Then, the approximate eigenfunctions of the electrons in the νth band are[37–39]

$$\varphi_{\nu\lambda;m}(\mathbf{r}) = \sum_l \tilde{\varphi}_{\nu\lambda;l}(\mathbf{r}) u_{\nu l;m}(\mathbf{r}), \tag{18}$$

where we have neglected the class B components, which do not change the symmetry. The slowly varying functions $\tilde{\varphi}_{\nu\lambda;l}(\mathbf{r})$ are the eigenfunctions of an effective-mass (Luttinger) Hamiltonian, which may include the modulations of the band edges in form of effective potentials and external fields.[37–39] Generally, we shall use the tilde to denote quantities in the effective-mass approximation.

The goal of the effective-mass approximation is to treat electrons in crystals like real electrons and to work only with the slowly varying envelope functions, while the properties of the lattice-periodic functions are condensed in a few matrix elements. Taking into account the strong localization of the function I, we can separate between slowly and rapidly varying parts and the effective Hamiltonian (16) goes over into

$$\begin{aligned}\hat{H}_{\text{ion-ion}} = -\frac{1}{2}\sum_{jj'} \sum_{\nu\lambda\nu'\lambda'} \frac{f_{\nu\lambda} - f_{\nu'\lambda'}}{E_{\nu'\lambda'} - E_{\nu\lambda}} \\ \times \hat{\mathbf{S}}_j \cdot \sum_{l_1 l_1'} \tilde{\varphi}^*_{\nu\lambda;l_1}(\mathbf{R}_j) \mathbf{I}_{\nu l_1,\nu' l_1'} \tilde{\varphi}_{\nu'\lambda';l_1'}(\mathbf{R}_j) \\ \times \sum_{l_2 l_2'} \tilde{\varphi}^*_{\nu'\lambda';l_2'}(\mathbf{R}_{j'}) \mathbf{I}_{\nu' l_2',\nu l_2} \tilde{\varphi}_{\nu\lambda;l_2}(\mathbf{R}_{j'}) \cdot \hat{\mathbf{S}}_{j'},\end{aligned} \tag{19}$$

where we assumed that $j \neq j'$. The matrix elements

$$\mathbf{I}_{\nu l,\nu' l'} = \sum_{mm'} \int d^3\mathbf{r} u^*_{\nu l;m}(\mathbf{r}) \mathbf{s}_{mm'} I(\mathbf{r}) u_{\nu' l';m'}(\mathbf{r}) \tag{20}$$

can be traced back to a few constants (the so-called exchange integrals α and β), which are determined experimentally[1] or by *ab initio* pseudopotential methods.[40] In optically excited or doped semiconductors, the intraband contributions ($\nu = \nu'$) are the dominating ones, because of the energy denominator in expression (19).

For the Γ_6 conduction and the Γ_8 valence band of a zinc-blende semiconductor, crystal symmetry requires the coupling matrix elements to be of the form

$$\mathbf{I}_{cl,cl'} = -I_c \frac{\sigma_{ll'}}{2}, \quad \mathbf{I}_{vl,vl'} = -I_v \mathbf{J}_{ll'}, \tag{21}$$

where $\mathbf{J} = (J_x, J_y, J_z)^T$ are the four-dimensional angular-momentum matrices, the so-called J matrices.

Comparing expressions (19) and (16), it appears that in the effective-mass approximation the conduction and valence electrons interact with the magnetic ions via an effective spin-orbit interaction of the form $-I_c \delta(\mathbf{r}-\mathbf{R}_j)\frac{\sigma}{2}\cdot\hat{\mathbf{S}}_j$ and $-I_v \delta(\mathbf{r}-\mathbf{R}_j)\mathbf{J}\cdot\hat{\mathbf{S}}_j$, respectively.[3] This effective interaction depends on the band indices and is proportional to a delta function—on the length scale of the slowly varying envelope functions. The coefficients I_c and I_v are related to the exchange integrals α and β by[1]

$$I_c = \frac{\alpha}{\hbar}, \quad I_v = \frac{\beta}{3\hbar}. \tag{22}$$

For the Γ_6 conduction band, the dispersion is parabolic and one can easily derive analytical expressions. For the Γ_8 valence band, the eigenfunctions $\tilde{\varphi}_{v\lambda}$ are four-component spinors, which need to be calculated numerically. This is, in principle, possible. However, to take advantage of the analytical results for the conduction band, it is common to neglect the contribution of the light hole and assume a parabolic dispersion for the heavy hole. The effective spin-orbit interaction of the heavy hole then has the form $-I_{\text{hh}}\delta(\mathbf{r}-\mathbf{R}_j)\frac{\sigma}{2}\cdot\mathbf{S}_j$, with

$$I_{\text{hh}} = 3I_v = \frac{\beta}{\hbar}. \tag{23}$$

B. Twofold degenerate band

The effective-mass Hamiltonian of a twofold degenerate band in the presence of structural confinement and external fields is

$$\hat{\tilde{H}} = \frac{1}{2m^*}\left[\frac{\hbar}{i}\nabla \mp e\mathbf{A}_{\text{ext}}(\mathbf{r})\right]^2 \pm eU_{\text{ext}}(\mathbf{r}) + W(\mathbf{r}) + \hat{\tilde{H}}_{\text{mag}}, \tag{24}$$

where $m^* = m_e, m_{\text{hh}}$ is the effective mass of the particle, $\mp e$ its charge, U_{ext} and $\mathbf{A}_{\text{ext}}$ are the scalar and the vector poten-

tial, and W is a potential characterizing the modulation of the band edge in a heterostructure.

The magnetic Hamiltonian $\hat{\tilde{H}}_{\mathrm{mag}}$ is determined by the interaction of the Bloch electron with the magnetic field, which is characterized by an intrinsic g factor g^*, and by the spin-orbit interaction with the magnetic ions. Introducing the magnetization of the ion spins,

$$\mathbf{M}(\mathbf{R}_j) = -\mu_0 \frac{x}{\Omega_0} \frac{g_{\mathrm{ion}} e}{2m_0} \langle \hat{\mathbf{S}}_j \rangle, \tag{25}$$

which is assumed to be a slowly varying function of $\mathbf{R}_j$, the magnetic Hamiltonian in the virtual crystal approximation (VCA) is given by

$$\hat{\tilde{H}}_{\mathrm{mag}} = \frac{g^* e}{2m_0} \mathbf{B}_{\mathrm{ext}}(\mathbf{r}) \cdot \mathbf{s} + \frac{1}{\mu_0} \frac{2m_0}{g_{\mathrm{ion}} e} \frac{I}{\hbar} \mathbf{M}(\mathbf{r}) \cdot \mathbf{s}, \tag{26}$$

where I is either $I_e = I_c$ or $I_{\mathrm{hh}} = 3I_v$ for the electron or heavy hole, respectively. In DMS, the contribution from the intrinsic g factor is negligible.

We assume $\mathbf{B}_{\mathrm{ext}} = B_{\mathrm{ext}}\, \mathbf{e}_z = \mathrm{const}$. Then the spin projection l is a good quantum number and the eigenvalues and eigenfunctions take the form

$$E_\lambda = E_{\mu m}, \quad E_{\mu\uparrow} - E_{\mu\downarrow} = \Delta E = \frac{1}{\mu_0} \frac{2m_0}{g_{\mathrm{ion}} e} IM$$

$$\tilde{\varphi}_{\lambda;l}(\mathbf{r}) = \tilde{\varphi}_{\mu m;l}(\mathbf{r}) = \tilde{\varphi}_\mu(\mathbf{r})\, \delta_{ml}, \tag{27}$$

and the effective Hamiltonian (19) becomes

$$\hat{H}_{\text{ion-ion}} = -\frac{1}{2} I^2 \sum_{jj'} \sum_{\mu\mu'} \sum_{mm'} \frac{f_{\mu m} - f_{\mu' m'}}{E_{\mu' m'} - E_{\mu m}} \hat{\mathbf{S}}_j \cdot \tilde{\varphi}^*_\mu(\mathbf{R}_j) \times \frac{\sigma_{mm'}}{2} \tilde{\varphi}_{\mu'}(\mathbf{R}_j) \tilde{\varphi}^*_{\mu'}(\mathbf{R}_{j'}) \frac{\sigma_{m'm}}{2} \tilde{\varphi}_\mu(\mathbf{R}_{j'}) \cdot \hat{\mathbf{S}}_{j'}. \tag{28}$$

In order to show the connection to the RKKY theory for free electrons,[18–20,22] it is instructive to consider the case that Zeeman splitting is negligible, i.e., $E_{\mu\uparrow} = E_{\mu\downarrow} = E_\mu$. Then, because of $\mathrm{Tr}(\sigma_\alpha \sigma_{\alpha'}) = 2\delta_{\alpha\alpha'}$, the effective Hamiltonian has the form of a Heisenberg Hamiltonian,

$$\hat{H}_{\text{ion-ion}} = -\frac{1}{2} \sum_{jj'} \Phi(\mathbf{R}_j, \mathbf{R}_{j'}) \hat{\mathbf{S}}_j \cdot \hat{\mathbf{S}}_{j'}, \tag{29}$$

where

$$\begin{aligned} \Phi(\mathbf{r}, \mathbf{r}') &= \frac{I^2}{2} \sum_{\mu\mu'} \frac{f_\mu - f_{\mu'}}{E_{\mu'} - E_\mu} \tilde{\varphi}^*_\mu(\mathbf{r}) \tilde{\varphi}_{\mu'}(\mathbf{r}) \tilde{\varphi}^*_{\mu'}(\mathbf{r}') \tilde{\varphi}_\mu(\mathbf{r}') \\ &= \frac{I^2}{2} \sum_{\mu\mu'} \frac{f_\mu (1 - f_{\mu'})}{E_{\mu'} - E_\mu} [\tilde{\varphi}^*_\mu(\mathbf{r}) \tilde{\varphi}_{\mu'}(\mathbf{r}) \tilde{\varphi}^*_{\mu'}(\mathbf{r}') \tilde{\varphi}_\mu(\mathbf{r}') \\ &\quad + \tilde{\varphi}^*_\mu(\mathbf{r}') \tilde{\varphi}_{\mu'}(\mathbf{r}') \tilde{\varphi}^*_{\mu'}(\mathbf{r}) \tilde{\varphi}_\mu(\mathbf{r})]. \end{aligned} \tag{30}$$

In case of translational invariance, the interaction matrix elements are of the form $\Phi(\mathbf{r}, \mathbf{r}') = \Phi(\mathbf{r} - \mathbf{r}')$. Then, the Fourier transform of Φ, known as the range function, is defined as

$$F(\mathbf{q}) = \int d^3\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} \Phi(\mathbf{r}). \tag{31}$$

Analogous definitions apply in two and one dimension.

For a Fermi sea of three-, two-, and one-dimensional free electrons, where the eigenfunctions are plane waves, the range function has been evaluated and the result is[22]

$$F_3(q) = \frac{I^2}{2} \frac{m^*}{4\pi^2\hbar^2} \frac{1}{q} \left[q k_F + \left(k_F^2 - \frac{q^2}{4} \right) \ln \left| \frac{q + 2k_F}{q - 2k_F} \right| \right]$$

$$F_2(q_\rho) = \frac{I^2}{2} \frac{m^*}{2\pi\hbar^2} \begin{cases} 1 & \text{for } q_\rho \leqslant 2k_F \\ 1 - \sqrt{1 - \left(\dfrac{2k_F}{q_\rho} \right)^2} & \text{for } q_\rho > 2k_F \end{cases}$$

$$F_1(q_z) = \frac{I^2}{2} \frac{m^*}{\pi\hbar^2} \frac{1}{q_z} \ln \left| \frac{q_z + 2k_F}{q_z - 2k_F} \right|, \tag{32}$$

where $k_F = \sqrt{2m^* E_F}/\hbar$ is the Fermi wave number and E_F is the Fermi energy. Taking F_1 as function of two variables $q_z \in \mathbb{R}$ and $k_F \in \mathbb{C}$, it has the obvious properties $F_1(-q_z, k_F) = F_1(q_z, k_F)$, $F_1(q_z, -k_F) = -F_1(q_z, k_F)$, $F_1(q_z; k_F^*) = F_1(q_z; k_F)$, and $F_1(q_z; k_F) = 0$ for $k_F \in i\mathbb{R}$. The Fourier transforms of the functions (32) are[22–25]

$$\Phi_3(r) = \frac{I^2}{2} \frac{m^*}{16\pi^3\hbar^2} \frac{\sin(2k_F r) - 2k_F r \cos(2k_F r)}{r^4},$$

$$\Phi_2(\rho) = -\frac{I^2}{2} \frac{m^* k_F^2}{4\pi\hbar^2} [J_0(k_F\rho) N_0(k_F\rho) + J_1(k_F\rho) N_1(k_F\rho)],$$

$$\Phi_1(z) = \frac{I^2}{2} \frac{m^*}{\pi\hbar^2} \left(\frac{\pi}{2} - \mathrm{Si}|2k_F z| \right). \tag{33}$$

The above expressions are for $T = 0$; the generalization to finite temperatures can be done by means of relation (17).

In contrast to the ideal d-dimensional electron gas, a realistic d-dimensional semiconductor has $3\text{-}d$ additional directions of confined motion. In this case the function Φ (30) depends on two three-dimensional vectors $\mathbf{r}$ and $\mathbf{r}'$, but translational invariance is fulfilled only for the d directions of free motion. Suppose that only the lowest subband $n = 0$ is occupied. Then one readily obtains for the RKKY interaction:[3]

$$\Phi(\mathbf{r}, \mathbf{r}') = |\tilde{\varphi}_0(\mathbf{r}_\perp)|^2 |\tilde{\varphi}_0(\mathbf{r}'_\perp)|^2 \Phi_d(\mathbf{r}_\parallel - \mathbf{r}'_\parallel; k_{F,0}), \tag{34}$$

where $\mathbf{r}_\perp$ and $\mathbf{r}_\parallel$ denote the directions of confined and free motion, respectively, and $\tilde{\varphi}_0$ is the ground-state wave function of the confined motion. In the expression for Φ_d (33), the Fermi wave number has to be replaced by $k_{F,0} = \sqrt{2m^*(E_F - E_0)}/\hbar$, where E_0 is the ground-state energy. For more complicated geometries or in the presence of interface roughness, it is desirable to directly calculate Φ from the

effective Hamiltonian (24). Such numerical methods have been proposed recently by Roche.[41]

The above considerations are valid only for geometrically low-dimensional semiconductors, where the confinement is caused by the modulation of the band edges, modeled by the function W in Eq. (24). The situation is more complicated if the dimensionality is reduced by a magnetic field. Actually, in this case, there is no unique definition of the dimensionality. From the point of translational symmetry, a bulk semiconductor in a magnetic field is three dimensional, whereas the $1/\sqrt{E}$ singularities in the density of states indicate one-dimensional behavior. Formula (34) is not applicable in this case, because the Landau levels have an infinite degeneracy. The form of Φ (34) is also in contradiction to the translational invariance of a bulk semiconductor in a magnetic field. As the density of states in a magnetic field is a series of one-dimensional densities of states, there is hope to express the range function as a series of one-dimensional range functions. In the next section, we calculate the range function for a three- and two-dimensional semiconductor in a magnetic field.

IV. SEMICONDUCTOR IN A MAGNETIC FIELD

In this section, we calculate the RKKY interaction of a semiconductor in a homogeneous magnetic field. We start with the three- and two-dimensional semiconductor, in case that the Zeeman splitting of the conduction band is negligible. Then the results are generalized to take into account Zeeman splitting.

A. Bulk semiconductor

We first neglect the Zeeman splitting so that $\hat{H}_{\text{ion-ion}}$ is of the form (29). A bulk semiconductor in a magnetic field is spatially homogeneous, even though this property is not reflected by the form of the vector potential. Here, we use the Landau gauge, $\mathbf{A}_{\text{ext}}(\mathbf{r})=B_{\text{ext}}x\mathbf{e}_y$, and, without loss of generality, assume that $B_{\text{ext}}>0$. Then, the explicit form of the eigenfunctions entering Eq. (30) is[42]

$$\tilde{\varphi}_\mu(\mathbf{r})=\tilde{\varphi}_{nk_yk_z}(\mathbf{r})=\frac{1}{\sqrt{L_z}}e^{ik_zz}\frac{1}{\sqrt{L_y}}e^{ik_yy}w_n\left(x\pm\frac{\hbar k_y}{eB_{\text{ext}}}\right),$$

$$w_n(x)=\frac{1}{\sqrt{\lambda_{\text{mag}}}}h_n\left(\frac{x}{\lambda_{\text{mag}}}\right),\quad h_n(\xi)=\frac{(-1)^n}{\sqrt{2^n n!\sqrt{\pi}}}e^{-\xi^2/2}H_n(\xi), \tag{35}$$

$$E_\mu=E_n(k_z)=\hbar\omega_c\left(n+\frac{1}{2}\right)+\frac{\hbar^2k_z^2}{2m^*},\quad n\in\mathbb{N}_0,\quad k_{y,z}\in\frac{2\pi\mathbb{Z}}{L_{y,z}},$$

where $\lambda_{\text{mag}}=\sqrt{\hbar/(eB_{\text{ext}})}$ is the magnetic length, $\omega_c=eB_{\text{ext}}/m^*$ is the cyclotron frequency, H_n denotes the Hermite polynomials, and L_y and L_z are the normalization lengths in the y and z direction, respectively. The energies are defined relative to the conduction-band edge and the occupation numbers for $T=0$ are $f_\mu=\Theta(E_F-E_\mu)$.

Inserting the solutions (35) into the second formulation in Eq. (30), the range function (31) becomes

$$F(\mathbf{q})=\frac{I^2}{2}\sum_{n=0}^{\infty}\sum_{n'=0}^{\infty}\frac{M_{nn'}(\lambda_{\text{mag}}q_\rho)}{(2\pi\lambda_{\text{mag}})^2}\int_{-\infty}^{+\infty}dk_z'\int_{-\infty}^{+\infty}dk_z'\times\frac{\Theta[E_F-E_n(k_z)]\Theta[E_{n'}(k_z')-E_F]}{\hbar\omega_c(n'-n)+\frac{\hbar^2}{2m^*}(k_z'^2-k_z^2)}\times[\delta(k_z'-k_z-q_z)+\delta(k_z'-k_z+q_z)], \tag{36}$$

where $q_\rho=\sqrt{q_x^2+q_y^2}$ and (Ref. 43, 7.377)

$$\begin{aligned}M_{nn'}(\sqrt{\alpha^2+\beta^2})&=M_{n'n}(\sqrt{\alpha^2+\beta^2})\\&=\left|\int_{-\infty}^{+\infty}d\xi e^{-i\alpha\xi}h_n(\xi)h_{n'}(\xi\pm\beta)\right|^2\\&=\frac{n'!}{n!}\left(\frac{\alpha^2+\beta^2}{2}\right)^{n-n'}e^{-\alpha^2+\beta^2/2}\times\left[L_{n'}^{(n-n')}\left(\frac{\alpha^2+\beta^2}{2}\right)\right]^2\\&=A_{nn'}\left(\frac{\alpha^2+\beta^2}{2}\right)\\&=A_{n'n}\left(\frac{\alpha^2+\beta^2}{2}\right)\end{aligned} \tag{37}$$

for $n\geqslant n'$. Here, $L_n^{(\alpha)}$ for $n\in\mathbb{N}_0$ and $\alpha>-1$ denote the generalized Laguerre polynomials, defined in Refs. 43 and 44, not to be confused with the associated Laguerre functions, often used in physics textbooks.[42] The $L_n^{(\alpha)}$ can be analytically continued to arbitrary complex α.[44] Then the above formula is valid also for $n<n'$. The coefficients $A_{nn'}$ are often used in the theory of the electron gas in a magnetic field.[45–49]

For the integration limits in Eq. (36) we find

$$\begin{aligned}\sum_{n=0}^{\infty}\int_{-\infty}^{+\infty}dk_z\Theta[E_F-E_n(k_z)]\cdots&=\sum_{n=0}^{\bar{n}}\int_{-k_{F,n}}^{+k_{F,n}}dk_z\cdots\sum_{n'=0}^{\infty}\int_{-\infty}^{+\infty}dk_z'\Theta[E_{n'}(k_z)-E_F]\cdots\\&=\sum_{n'=0}^{\infty}\int_{-\infty}^{+\infty}dk_z'\cdots-\sum_{n'=0}^{\bar{n}}\int_{-k_{F,n'}}^{+k_{F,n'}}dk_z'\cdots,\end{aligned} \tag{38}$$

where $\bar{n}$ is the highest occupied Landau level, i.e., the largest integer with $E_{\bar{n}}(0)<E_F$, and

$$k_{F,n} = \frac{\sqrt{2m^*}}{\hbar}\sqrt{E_F - \hbar\omega_c\left(n+\frac{1}{2}\right)} \tag{39}$$

is the Fermi wave number of the nth Landau level. For reasons which become clear below we shall also consider imaginary $k_{F,n}$, which occur for $n > \bar{n}$.

The second k_z' integral in Eq. (38) vanishes for symmetry reasons and the remaining integrals have to be interpreted as principal values. The rest of the calculation is straightforward and the result is

$$F(\mathbf{q}) = \frac{I^2}{2}\sum_{n=0}^{\bar{n}}\sum_{n'=0}^{\infty}\frac{M_{nn'}(\lambda_{\mathrm{mag}}q_\rho)}{2\pi\lambda_{\mathrm{mag}}^2}\frac{m^*}{\pi\hbar^2 q_z} \times\ln\left|\frac{\hbar\omega_c(n'-n)+(\hbar^2/2m^*)q_z(q_z+2k_{F,n})}{\hbar\omega_c(n'-n)+(\hbar^2/2m^*)q_z(q_z-2k_{F,n})}\right|. \tag{40}$$

This is the range function of a three-dimensional semiconductor in a magnetic field. The result is equivalent to the expression for the random-phase approximation (RPA) polarization function of a three-dimensional electron gas in a magnetic field obtained by Schulz and Keiter.[45]

It is instructive to write expression (40) in a different way. The q_z-dependent parts closely resemble the range function F_1 (32). From

$$\hbar\omega(n'-n) = \frac{\hbar^2}{2m^*}(k_{F,n}^2 - k_{F,n'}^2)$$

it follows that

$$\ln\left|\frac{\hbar\omega_c(n'-n)+(\hbar^2/2m^*)q_z(q_z+2k_{F,n})}{\hbar\omega_c(n'-n)+(\hbar^2/2m^*)q_z(q_z-2k_{F,n})}\right| = \ln\left|\frac{q_z+(k_{F,n}+k_{F,n'})}{q_z-(k_{F,n}+k_{F,n'})}\right| + \ln\left|\frac{q_z+(k_{F,n}-k_{F,n'})}{q_z-(k_{F,n}-k_{F,n'})}\right|$$

and, therefore,

$$F(\mathbf{q}) = \sum_{n=0}^{\bar{n}}\sum_{n'=0}^{\infty}\frac{M_{nn'}(\lambda_{\mathrm{mag}}q_\rho)}{2\pi\lambda_{\mathrm{mag}}^2} \times\left[F_1\left(q_z;\frac{k_{F,n}+k_{F,n'}}{2}\right)+F_1\left(q_z;\frac{k_{F,n}-k_{F,n'}}{2}\right)\right].$$

Using the analytical properties of $F_1(q_z;k_F)$, we can finally write the range function in the symmetric form

$$F(\mathbf{q}) = \sum_{n=0}^{\infty}\sum_{n'=0}^{\infty}\frac{M_{nn'}(\lambda_{\mathrm{mag}}q_\rho)}{2\pi\lambda_{\mathrm{mag}}^2}F_1\left(q_z;\frac{k_{F,n}+k_{F,n'}}{2}\right). \tag{41}$$

If $n > \bar{n}$ and $n' > \bar{n}$, then the contribution to the sum is zero, because the second argument of F_1 is purely imaginary. As F_1 has a logarithmic singularity if and only if the Fermi wave number is real, the function (41) has $(\bar{n}+1)(\bar{n}+2)/2$ logarithmic singularities in the region $0 < q_z < 2k_F$, where k_F is the three-dimensional Fermi wave number. In the limit $B_{\mathrm{ext}} \to 0$, one expects $F(\mathbf{q})$ to go over into the three-dimensional range function $F_3(q;k_F)$ (32).

For the graphic representation, we use dimensionless quantities, defined by $I^2/2 = \hbar = e = m^* = 1$. To visualize the dependence on q_ρ and q_z, we introduce the radial coordinate $q = |\mathbf{q}|$ and the azimuthal angle θ with $q_z = q\cos\theta$ and $q_\rho = q\sin\theta$. In Fig. 1, the range function F of a three-dimensional semiconductor in a magnetic field (40) is shown for a Fermi energy $E_F = 1/2$, corresponding to a three-dimensional Fermi wave number $k_F = \sqrt{2E_F} = 1$, and various magnetic-field strengths $B_{\mathrm{ext}} = 1/2$, $B_{\mathrm{ext}} = 1/10$, and $B_{\mathrm{ext}} = 1/50$, corresponding to 1, 5, and 25 Landau levels below the Fermi level. The results are compared with the three-dimensional range function F_3 (32).

For $\theta = 0$, the radius q coincides with the coordinate q_z and the radial coordinate q_ρ is equal to zero. In this case, as $M_{nn'}(0) = 0$ for $n \neq n'$, only terms with $n = n'$ contribute to $F(q_\rho = 0, q_z)$. For a large magnetic field, $B_{\mathrm{ext}} = 0.5$, we observe a strong peak at $q_z = 2k_{F,0} = \sqrt{2}$. If B_{ext} is reduced at constant Fermi energy, more Landau levels become occupied, each one leading to a logarithmic singularity in the interval $q_z \in (0, 2k_F)$. The weight of the singularities decreases as B_{ext} decreases and the range function converges towards the three-dimensional range function F_3. This function does not have any singularities, but is nonanalytic at $q = 2k_F$, as seen from Eq. (32). There are no singularities in the region $q_z > 2k_F$ for any B_{ext} and the range function closely resembles the three-dimensional limit F_3 even for large fields.

For $\theta \neq 0$, the singularities are located at $q_n = k_{F,n}/\cos\theta = \sqrt{1 - B_{\mathrm{ext}}(2n+1)}/\cos\theta$ for $n = 0, \ldots, \bar{n}$, but their magnitudes are considerably smaller than for $\theta = 0$. Furthermore, as $q_\rho > 0$, the sum does now include contributions also for $n' \neq n$, which leads to additional logarithmic singularities and a fairly irregular structure. This is clearly observable for $B_{\mathrm{ext}} = 0.1$ at $\theta = 30°$ and $\theta = 60°$. For $\theta > 0$, there are also singularities in the region $q > 2k_F$, but their height is vanishingly small so that they cannot be seen by eye.

An azimuthal angle $\theta = 90\circ$ corresponds to $q_z = 0$ and $q = q_\rho$. There are no singularities in this direction, but each Landau level leads to a local maximum of the function F. There is one maximum for $B_{\mathrm{ext}} = 0.5$, five maxima for $B_{\mathrm{ext}} = 0.1$, and 25 maxima for $B_{\mathrm{ext}} = 0.02$. For all angles θ, the range function F converges towards F_3 as B_{ext} goes to zero.

For any finite temperature, the logarithmic singularities disappear, because of the integral kernel of width $k_B T$ (17). This was noticed in the early papers on the dielectric response of a three-dimensional electron gas in a magnetic field.[45,47] In the limit $k_B T \gg \hbar\omega_c$, which is of practical interest, the sum over the quantum number n can be approximated by an integral over the continuous variable k_ρ, and the result is the same as for $B_{\mathrm{ext}} = 0$. Furthermore, for $B = 0$, the effect of the finite temperature is relatively small due to the smoothness of $F_3(q)$ (cf. Fig. 1). Consequently, for $k_B T \gg \hbar\omega_c$, the range function can be approximated as $F(\mathbf{q};B,T) \approx F_3(q;B=0,T=0)$.

We are now ready to study the case that only the lowest Landau level is occupied. Then in expression (40) the first sum is restricted to $n = 0$. Obviously, this is not a major simplification, because the n' sum still runs from 0 to ∞. Only in the limit $\hbar^2 k_{F,0}^2/(2m^*) \ll \hbar\omega_c$ or, equivalently, $E_F - \frac{1}{2}\hbar\omega_c \ll \hbar\omega_c$, the terms with $n' > 0$ can be neglected and formula (41) simplifies to

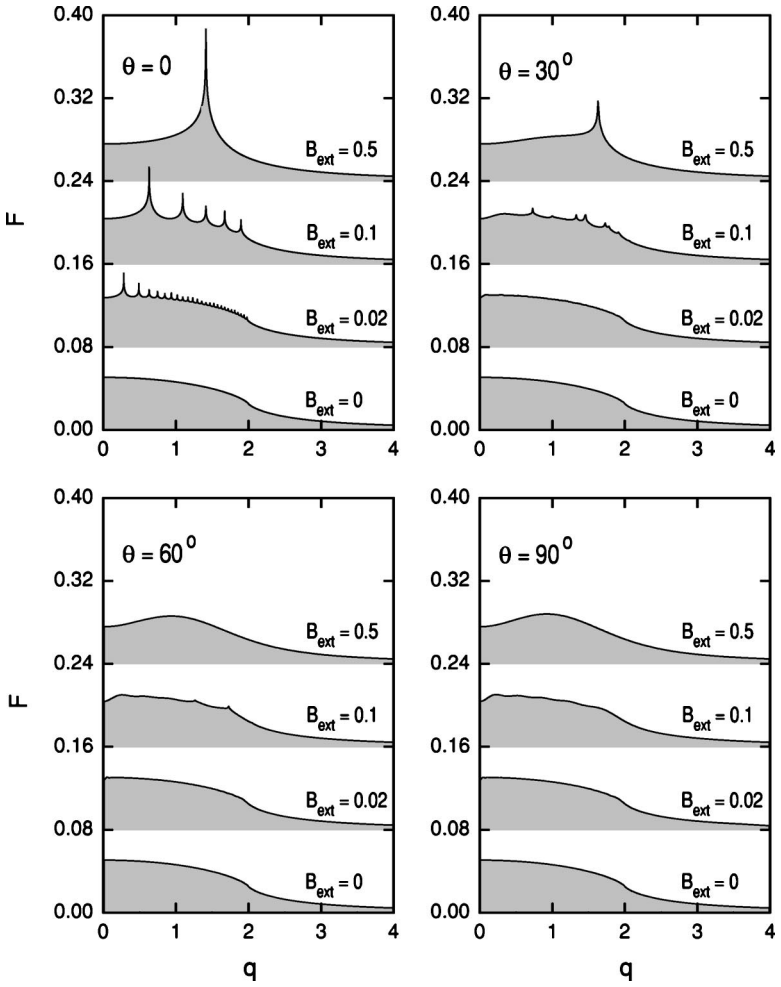

FIG. 1. Range function F of a three-dimensional semiconductor in a magnetic field as a function of q for $E_F=\frac{1}{2}$ and $B_{\text{ext}}=0.5$, 0.1, 0.02, and $B_{\text{ext}}=0$, corresponding to the three-dimensional range function F_3 (32). The azimuthal angle is $\theta=0$ ($q=q_z$), 30°, 60°, and 90° ($q=q_\rho$).

$$F(\mathbf{q}) = \frac{1}{2\pi\lambda_{\text{mag}}^2}\exp\left(-\frac{\lambda_{\text{mag}}^2 q_\rho^2}{2}\right)F_1(q_z;k_{F,0}). \qquad (42)$$

For the largest field in Fig. 1, the above approximation perfectly agrees with the exact solution. The RKKY interaction in real space is given by Fourier transform of expression (42) and the result is

$$\Phi(\mathbf{r}) = \frac{1}{(2\pi\lambda_{\text{mag}}^2)^2}\exp\left(-\frac{\rho^2}{2\lambda_{\text{mag}}^2}\right)\Phi_1(z;k_{F,0}), \qquad (43)$$

with Φ_1 defined in Eq. (33). We see that there is no way of writing the expression (43) in the form (34). The extension of the function (43) in the plane perpendicular to the magnetic field is in the order of the magnetic length $\lambda_{\text{mag}}=\sqrt{\hbar/(eB_{\text{ext}})}$, and is independent of the density. In the z direction, Φ shows an oscillating behavior with period $\pi/k_{F,0}=1/(\pi\varrho\lambda_{\text{mag}}^2)$. This means that for a constant density ϱ the extension of Φ in the field direction is proportional to the magnetic field.

B. Two-dimensional semiconductor

To calculate the range function of a two-dimensional semiconductor in a magnetic field, we only need to drop the z direction in Eq. (36), and the resulting range function is

$$F(\mathbf{q}_\parallel) = F'(\mathbf{q}_\parallel) + F''(\mathbf{q}_\parallel),$$

$$F'(\mathbf{q}_\parallel) = \frac{I^2}{2}\sum_{n=0}^{\infty}\frac{M_{nn}(\lambda_{\text{mag}}q_\rho)}{2\pi\lambda_{\text{mag}}^2}\left.\frac{-df(E)}{dE}\right|_{E=E_n},$$

$$F''(\mathbf{q}_\parallel) = \frac{I^2}{2}\sum_{n=0}^{\infty}\sum_{n'=0}^{\infty}\frac{M_{nn'}(\lambda_{\text{mag}}q_\rho)}{2\pi\lambda_{\text{mag}}^2}\frac{f(E_n)-f(E_{n'})}{E_{n'}-E_n}. \qquad (44)$$

Here we give the general expression for $T\geqslant 0$ because of the divergence for $T=0$. The function F' contains only the diagonal contributions ($n=n'$) and the limit $0/0$ is replaced by the derivative of the Fermi function. The nondiagonal contributions are contained in F'', where the sum is carried out only for $n\neq n'$. The result (44) is identical to the expression for the polarization function in RPA found by Gerhards and Gudmundsson.[48]

The function F'' (44) for $T=0$ is shown in Fig. 2 for the same parameters as in Fig. 1. For $B_{\text{ext}}>0$, this function has $\overline{n}+1$ clear and distinct maxima in the region $q_\rho\in(0,2k_F)$. In the limit $q_\rho\to\infty$, F'' rapidly converges towards F_2 (lowest curve) for any B_{ext}. In fact, for $q_\rho\geqslant 3$, the solutions for finite B_{ext} are virtually indistinguishable from the solution for $B_{\text{ext}}=0$. The behavior of F in the neighborhood of $q_\rho=2k_F=2$ for small B_{ext} can be compared to the Gibbs phenomenon

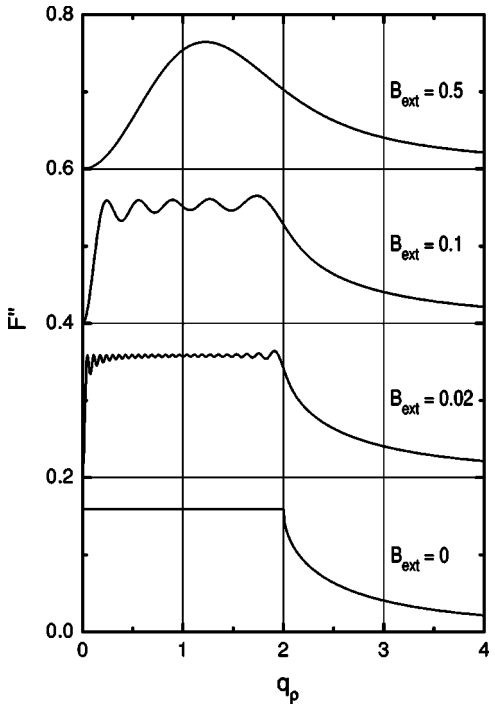

FIG. 2. Nondiagonal range function F'' at $T=0$ of a two-dimensional semiconductor in a magnetic field as function of the in-plane wave number q_ρ for $E_F=\frac{1}{2}$ and $B_{\text{ext}}=0.5$, 0.1, 0.02, and $B_{\text{ext}}=0$, corresponding to the two-dimensional range function F_2 (32).

known from Fourier series. Nonuniform convergence is observed also for $q_\rho=0$: the value of $F_2(0)$ is $m/(2\pi\hbar^2)$, while $F''(\mathbf{q}_\parallel=0)=0$.

For $B_{\text{ext}}\neq 0$, the function F' becomes divergent for $T=0$, because the derivative of the Fermi function is $-df(E)/dE = \delta(E-E_F)$. However, for $B_{\text{ext}}\to 0$, $T\to 0$, $\hbar\omega_c/(k_BT)\to 0$ we have

$$F'(\mathbf{q}_\rho)\to\begin{cases}\dfrac{I^2}{2}\dfrac{m^*}{2\pi\hbar^2} & \text{for } q_\rho=0\\ 0 & \text{for } q_\rho>0.\end{cases}$$

In this limit the function F (44) converges towards the two-dimensional range function F_2 (32).

For fixed density, in the limit $B_{\text{ext}}\to\infty$, only the lowest Landau level remains occupied and the contribution from F'' disappears. The RKKY interaction in real space is then proportional to the ρ-dependent part of expression (43), which does not show any oscillations.

Formula (44) is useful to describe the RKKY interaction of a quantum well in a perpendicular magnetic field in case that only the lowest well subband is occupied. The dropped z dependence can be included in analogy to formula (34).

C. Inclusion of Zeeman splitting

As result of the giant effective g factor, the Zeeman splitting is usually not negligible in DMS. In this case, one can no longer assume that the RKKY interaction is isotropic, and instead of Eq. (29) one has

$$\hat{H}_{\text{ion-ion}}=-\frac{1}{2}\sum_{jj'}\sum_{\alpha\alpha'}\hat{S}^\dagger_{j\alpha}\Phi_{\alpha\alpha'}(\mathbf{R}_j,\mathbf{R}_{j'})\hat{S}_{j'\alpha'}. \tag{45}$$

From general principles of magnetooptics,[50] one expects the eigenvectors of Φ to be $\mathbf{e}_+$, $\mathbf{e}_-$, and $\mathbf{e}_z$, where

$$\mathbf{e}_\pm=\frac{1}{\sqrt{2}}(\mathbf{e}_x\pm i\mathbf{e}_y)=\mathbf{e}^*_\mp$$

are the unit vectors for right- and left-circular polarization, known from the theory of the Faraday effect. Furthermore, it is convenient to transform also the spin operators and the Pauli matrices

$$\hat{S}_{j\pm}=\frac{1}{\sqrt{2}}(\hat{S}_{jx}\pm i\hat{S}_{jy})=\hat{S}^\dagger_{j\mp},\quad \sigma_\pm=\frac{1}{\sqrt{2}}(\sigma_x\pm i\sigma_y)=\sigma^\dagger_\mp.$$

(Note that in the quantum theory of angular momenta the definition usually does not include a factor $1/\sqrt{2}$.) Then, Eq. (45) is also valid in the new coordinates $+,-,z$.

For the Γ_6 band under consideration, according to Eq. (28), the matrix elements of Φ (45) are

$$\Phi_{\alpha\alpha'}(\mathbf{r},\mathbf{r}')=\frac{1}{2}\sum_{mm'}\Phi_{mm'}(\mathbf{r},\mathbf{r}')\sigma^\dagger_{\alpha mm'}\sigma_{\alpha' m'm}, \tag{46}$$

where

$$\Phi_{mm'}(\mathbf{r},\mathbf{r}')=\frac{I^2}{2}\sum_{\mu\mu'}\frac{f_{\mu m}-f_{\mu' m'}}{E_{\mu' m'}-E_{\mu m}}\tilde{\varphi}^*_\mu(\mathbf{r})\tilde{\varphi}_{\mu'}(\mathbf{r})\tilde{\varphi}^*_{\mu'}(\mathbf{r}')\tilde{\varphi}_\mu(\mathbf{r}'). \tag{47}$$

From the explicit expressions

$$\sigma_+=\begin{pmatrix}0&\sqrt{2}\\0&0\end{pmatrix},\quad \sigma_-=\begin{pmatrix}0&0\\\sqrt{2}&0\end{pmatrix}$$

we find that Φ is indeed diagonal in the new coordinates and the diagonal matrix elements are given by

$$\Phi_{++}(\mathbf{r},\mathbf{r}')=\Phi_{\uparrow\downarrow}(\mathbf{r},\mathbf{r}'),\quad \Phi_{--}(\mathbf{r},\mathbf{r}')=\Phi_{\downarrow\uparrow}(\mathbf{r},\mathbf{r}'),$$

$$\Phi_{zz}(\mathbf{r},\mathbf{r}')=\tfrac{1}{2}[\Phi_{\uparrow\uparrow}(\mathbf{r},\mathbf{r}')+\Phi_{\downarrow\downarrow}(\mathbf{r},\mathbf{r}')]. \tag{48}$$

The remaining task is to determine the Fourier transforms $F_{mm'}$ of the $\Phi_{mm'}$ (47). The eigenfunctions in the definition of $\Phi_{mm'}$ (47) are given in Eq. (35), and the energies, which include the Zeeman splitting, are

$$E_{n\uparrow,\downarrow}(k_z)=\hbar\omega_c\left(n+\frac{1}{2}\right)+\frac{\hbar^2k_z^2}{2m^*}\pm\frac{1}{2}\Delta E. \tag{49}$$

The rest of the calculation closely follows the derivation of the result (41), when Zeeman splitting was neglected. First, we carry out the k_x and k_y integrations, which leads us to

$$F_{mm'}(\mathbf{q}) = \frac{I^2}{2}\sum_{n=0}^{\infty}\sum_{n'=0}^{\infty}\frac{M_{nn'}(\lambda_{\mathrm{mag}}q_\rho)}{(2\pi\lambda_{\mathrm{mag}})^2}\int_{-\infty}^{+\infty}dk_z\int_{-\infty}^{+\infty}dk_z' \times\frac{\Theta[E_F-E_{nm}(k_z)]-\Theta[E_F-E_{n'm'}(k_z')]}{E_{n'm'}(k_z')-E_{nm}(k_z)} \times\delta(k_z'-k_z-q_z). \tag{50}$$

The function $\Theta[E_F-E_{nm}(k_z)]$ restricts the k_z integration to the interval $[-k_{F,nm},+k_{F,nm}]$, with $k_{F,nm}$ defined by

$$E_{nm}(0)+\frac{\hbar^2k_{F,nm}^2}{2m^*}=E_F, \tag{51}$$

and the summation to $n=0,\ldots,\overline{n_m}$, for which $k_{F,nm}$ is real. It is worthwhile to note that $\overline{n_\uparrow}$ may be different from $\overline{n_\downarrow}$, which means a different number of Landau levels inside the Fermi sphere for the spin-up and spin-down states.

Now the denominator in Eq. (50) can be expressed in terms of $k_{F,nm}$ and $k_{F,n'm'}$ (real or imaginary), the integrals can be carried out explicitly, and the resulting logarithms can be represented by one-dimensional range functions. The result of the calculation is

$$\begin{aligned}F_{mm'}(\mathbf{q}) = &\sum_{n=0}^{\overline{n_m}}\sum_{n'=0}^{\infty}\frac{M_{nn'}(\lambda_{\mathrm{mag}}q_\rho)}{4\pi\lambda_{\mathrm{mag}}^2}\left[F_1\left(q_z;\frac{k_{F,nm}+k_{F,n'm'}}{2}\right)\right.\\ &\left.+F_1\left(q_z;\frac{k_{F,nm}-k_{F,n'm'}}{2}\right)\right]\\ &+\sum_{n=0}^{\infty}\sum_{n'=0}^{\overline{n_{m'}}}\frac{M_{nn'}(\lambda_{\mathrm{mag}}q_\rho)}{4\pi\lambda_{\mathrm{mag}}^2}\left[F_1\left(q_z;\frac{k_{F,n'm'}+k_{F,nm}}{2}\right)\right.\\ &\left.+F_1\left(q_z;\frac{k_{F,n'm'}-k_{F,nm}}{2}\right)\right].\end{aligned} \tag{52}$$

If $\overline{n_m}=\overline{n_{m'}}$, which means that either $m=m'$ or $m\neq m'$ and $\overline{n_\uparrow}=\overline{n_\downarrow}$, the sums can be rearranged to give

$$F_{mm'}(\mathbf{q})=\sum_{n=0}^{\infty}\sum_{n'=0}^{\infty}\frac{M_{nn'}(\lambda_{\mathrm{mag}}q_\rho)}{2\pi\lambda_{\mathrm{mag}}^2}F_1\left(q_z;\frac{k_{F,nm}+k_{F,n'm'}}{2}\right), \tag{53}$$

where the contributions for $n,n'>\overline{n_m}=\overline{n_{m'}}$ are zero. The functions $F_{\uparrow\uparrow}$ and $F_{\downarrow\downarrow}$ are identical to the range function in the absence of Zeeman splitting (41), when the Fermi energy is replaced by $E_F\mp\frac{1}{2}\Delta E$.

For the system under consideration, we find that $F_{mm'}(\mathbf{q})=F_{m'm}(\mathbf{q})$ and, therefore, $F_{++}(\mathbf{q})=F_{--}(\mathbf{q})$. Thus, the RKKY interaction is diagonal also in Cartesian coordinates and is isotropic in the xy plane with $F_{xx}(\mathbf{q})=F_{yy}(\mathbf{q})=F_{\rho\rho}(\mathbf{q})$. Normally, F_{zz} is different from $F_{\rho\rho}$. In the limit $k_BT\gg\hbar\omega_c$, according to the discussion in Sec. IV A, it can be approximated by $F_{zz}(\mathbf{q})=\frac{1}{2}[F_3(q;E_F-\frac{1}{2}\Delta E)+F_3(q;E_F+\frac{1}{2}\Delta E)]$, where F_3 is the three-dimensional range function (32).

For the ideally two-dimensional semiconductor, the result, including Zeeman splitting, is

$$F_{mm'}(\mathbf{q}_\parallel)=\frac{I^2}{2}\sum_{n=0}^{\infty}\sum_{n'=0}^{\infty}\frac{M_{nn'}(\lambda_{\mathrm{mag}}q_\rho)}{2\pi\lambda_{\mathrm{mag}}^2}\frac{f(E_{nm})-f(E_{n'm'})}{E_{n'm'}-E_{nm}}. \tag{54}$$

Here, the result is given for finite temperature because of the divergency for $T\to0$. For $(n,m)=(n',m')$, the limit $0/0$ has to be replaced by the derivative $-df/dE$ at $E=E_{nm}$.

V. INFLUENCE OF SCREENING

The expressions (30) and (47) for the range function rely on two approximations, which are commonly found in the literature,[25–28] namely, (i) the density correlation function L is replaced by its irreducible part Π, which means that screening is neglected, and (ii) Π is approximated by $\Pi^{(0)}$, which contains no pair correlations. The spin susceptibility, including screening, was calculated decades ago by Kim *et al.*,[30] but these works are largely unnoticed in present publications on ferromagnetism in DMS.

Besides the approximations made in the calculation of the susceptibility, the RKKY theory is a perturbation theory, which relies on the smallness of the interaction Hamiltonian, in comparison to the energetic distance between ground and excited states. This approximation is never fulfilled if the spectrum of the electrons is continuous. Some authors express the exchange field in terms of the magnetization of the electrons,[3,5] which is called mean-field Zener theory and goes back to Stoner.[21] In this section we show that both approaches are equivalent when screening is included in the RKKY interaction.

A. Mean-field theory of ferromagnetism

The treatment of the ion-ion interaction is considerably simplified by means of mean-field theory, which reduces the many-particle problem to an effective one-particle problem. This allows to approximately calculate the magnetization and to estimate the Curie temperature. Here, we introduce the fundamental equations of mean-field theory.

The Hamiltonian of the magnetic ions in the presence of an external magnetic field is given by

$$\begin{aligned}\hat{H}_{\mathrm{ion}}&=\hat{H}_{\text{ion-ion}}+\hat{H}_{\text{ion-mag}}\\ &=-\frac{1}{2}\sum_{jj'}\sum_{\alpha\alpha'}\hat{S}_{j\alpha}\Phi_{\alpha\alpha'}(\mathbf{R}_j-\mathbf{R}_{j'})\hat{S}_{j'\alpha'}\\ &\quad+\frac{g_{\mathrm{ion}}e}{2m_0}\sum_j\sum_\alpha B_{\mathrm{ext}\,\alpha}(\mathbf{R}_j)\hat{S}_{j\alpha}.\end{aligned} \tag{55}$$

We assume that $\mathbf{B}_{\mathrm{ext}}(\mathbf{r})=B_{\mathrm{ext}}(\mathbf{r})\mathbf{e}_z$. In the mean-field approximation,[5] the expression (55) is replaced by an effective one-particle Hamiltonian

$$\hat{H}_{\mathrm{MF}}=\frac{g_{\mathrm{ion}}e}{2m_0}\sum_j\hat{S}_{jz}[B_{\mathrm{ext}}(\mathbf{R}_j)+B_{\mathrm{exc},j}]+\mathrm{const}, \tag{56}$$

where

$$B_{\mathrm{exc},j} = -\frac{2m_0}{g_{\mathrm{ion}}e}\sum_{j'}\Phi_{zz}(\mathbf{R}_j - \mathbf{R}_{j'})\langle\hat{S}_{j'z}\rangle \tag{57}$$

is the exchange field, which approximately describes the interaction of one magnetic ion with the background of the other magnetic ions. The constant in Eq. (56) is a scalar, which merely shifts the energy to zero and can be neglected. Formally, the mean-field Hamiltonian (56) describes a paramagnetic system in an effective field $B_{\mathrm{ext}}+B_{\mathrm{exc}}$. In the canonical ensemble, the expectation values for the spin projections are[51]

$$\langle\hat{S}_{jz}\rangle = -\hbar S\mathcal{B}_S\left\{\frac{\hbar S}{k_BT}\frac{g_{\mathrm{ion}}e}{2m_0}[B_{\mathrm{ext}}(\mathbf{R}_j) + B_{\mathrm{exc},j}]\right\}, \tag{58}$$

with the Brillouin function

$$\mathcal{B}_S(\xi) = \frac{2S+1}{2S}\coth\left(\frac{2S+1}{2S}\xi\right) - \frac{1}{2S}\coth\left(\frac{1}{2S}\xi\right). \tag{59}$$

The function $\mathcal{B}_S$ is monotonous and its derivative at $\xi=0$ is $(S+1)/(3S)$. The asymptotic behavior is $\mathcal{B}_S(\xi)\to\pm 1$ for $\xi\to\pm\infty$. As the exchange field $B_{\mathrm{exc},j}$ itself depends on the $\langle\hat{S}_{jz}\rangle$, Eqs. (57) and (58) have to be solved self-consistently.

We assume that B_{ext} is constant over the size of the sample. As Φ is slowly varying, compared with the lattice constant, the sum in Eq. (57) can be approximated by an integral over $d^3\mathbf{R}_{j'}$ times a factor x/Ω_0. With the definition of the magnetization (25), Eqs. (58) and (57) go over into

$$M = \mu_0\frac{x}{\Omega_0}\frac{g_{\mathrm{ion}}e}{2m_0}\hbar S\mathcal{B}_S\left\{\frac{\hbar S}{k_BT}\frac{g_{\mathrm{ion}}e}{2m_0}(B_{\mathrm{ext}} + B_{\mathrm{exc}})\right\} \tag{60}$$

and

$$B_{\mathrm{exc}} = \frac{1}{\mu_0}\left(\frac{2m_0}{g_{\mathrm{ion}}e}\right)^2 F_{zz}(0)M. \tag{61}$$

The system is called ferromagnetic if there exists a nontrivial solution $M\neq 0$ for $B_{\mathrm{ext}}=0$. This is the case for $T<T_C$ with the Curie temperature[3,52]

$$T_C = \frac{\hbar^2 S(S+1)}{3k_B}\frac{x}{\Omega_0}F_{zz}(0). \tag{62}$$

For a direct experimental measurement of ferromagnetism it is necessary that the magnetization on the account of paramagnetism is well below the saturation value. This is the case if for $B_{\mathrm{exc}}=0$ the value of the Brillouin function (60) is much smaller than unity, which requires that

$$\frac{g_{\mathrm{ion}}(S+1)}{6}\frac{\hbar eB}{m_0} \ll k_BT. \tag{63}$$

This also means that $\hbar\omega_c \ll k_BT$, especially for the heavy hole and, following the discussion in Sec. IV C, the effect of the magnetic field on the orbital motion can be neglected. In the following we shall restrict ourselves to this limit; the inclusion of the Landau quantization is straightforward.

B. The exchange field

We have seen that, in the mean-field approximation, the magnetization is determined by the integral over the RKKY interaction, which gives the range function at $\mathbf{q}=0$. As shown in Sec. II B, the RKKY interaction is related to the density correlation function (14). In the effective-mass approximation for a Kramers-degenerate band, considered in Sec. III B, these equations write

$$\Phi_{\alpha\alpha'}(\mathbf{r},\mathbf{r}') = \mu_0\left(\frac{m_0}{\mu_0 e}\right)^2 I^2\tilde{\chi}_{\mathrm{ret}\ \alpha\alpha'}(\mathbf{r},\mathbf{r}',\omega=0)$$
$$= -\frac{I^2}{2}\tilde{L}_{\mathrm{ret}\ \alpha\alpha'}(\mathbf{r},\mathbf{r}',\omega=0),$$

$$\tilde{L}_{\mathrm{ret}\ \alpha_1\alpha_2}(\mathbf{r}_1,\mathbf{r}_2,\omega) = \frac{1}{2}\sum_{m_1m_1'}\sum_{m_2m_2'}\sigma_{\alpha_1m_1'm_1}$$
$$\times\tilde{L}_{\mathrm{ret}\ m_1m_1',m_2m_2'}(\mathbf{r}_1,\mathbf{r}_2,\omega)\sigma_{\alpha_2m_2'm_2}. \tag{64}$$

Here $\tilde{\chi}$ and $\tilde{L}$ are the spin susceptibility and the density correlation function of an electron gas governed by the one-particle Hamiltonian (24) and subjected to Coulomb interaction.

The relation between $\tilde{L}$ and its irreducible part, the polarization function $\tilde{\Pi}$ is given by[35,36]

$$\tilde{L}_{\mathrm{ret}\ m_1m_1',m_2m_2'}(\mathbf{q},\omega) = \tilde{\Pi}_{\mathrm{ret}\ m_1m_1',m_2m_2'}(\mathbf{q},\omega)$$
$$+\sum_{m_3m_4}\tilde{\Pi}_{\mathrm{ret}\ m_1m_1',m_3m_3}(\mathbf{q},\omega)\tilde{v}(\mathbf{q})$$
$$\times\tilde{L}_{\mathrm{ret}\ m_4m_4,m_2m_2'}(\mathbf{q},\omega). \tag{65}$$

Here, the Coulomb interaction $\tilde{v}(\mathbf{q})=e^2/(\varepsilon_0\varepsilon q^2)$ statically screened by a dielectric constant $\varepsilon\approx 10$ through interaction with nonresonant bands (interband transitions). To rewrite the above equation for the functions $\tilde{L}_{\alpha\beta}$ and $\tilde{\Pi}_{\alpha\beta}$ (64), we also take into account the components $\alpha,\beta=0$, where $\sigma_0=\mathrm{diag}(1,1)$ is the two-dimensional unity matrix, and employ the orthonormality and completeness relations of the Pauli matrices

$$\frac{1}{2}\sum_{mm'}\sigma_{\alpha_1mm'}\sigma_{\alpha_2m'm} = \delta_{\alpha_1\alpha_2},$$

$$\frac{1}{2}\sum_{\alpha=0}^{4}\sigma_{\alpha m_1'm_1}\sigma_{\alpha m_2,m_2'} = \delta_{m_1m_2}\delta_{m_1'm_2'}. \tag{66}$$

The components $\alpha=0$ and $\alpha=1,2,3=x,y,z$ correspond to the singlet and triplet states of the two-particle system. In the new indices, Eq. (65) reads[36]

$$\tilde{L}_{\mathrm{ret}\,\alpha_1\alpha_2}(\mathbf{q},\omega) = \tilde{\Pi}_{\mathrm{ret}\,\alpha_1\alpha_2}(\mathbf{q},\omega) + \sum_{\alpha_3,\alpha_4=0}^{4} \tilde{\Pi}_{\mathrm{ret}\,\alpha_1\alpha_3}(\mathbf{q},\omega)\tilde{v}_{\alpha_3\alpha_4}(\mathbf{q})\tilde{L}_{\mathrm{ret}\,\alpha_4\alpha_2}(\mathbf{q},\omega) \tag{67}$$

with the transformed Coulomb potential

$$\tilde{v}_{\alpha_3\alpha_4}(\mathbf{q}) = \begin{cases} 2\tilde{v}(\mathbf{q}) & \text{for } \alpha_3=\alpha_4=0 \\ 0 & \text{elsewhere.} \end{cases} \tag{68}$$

Because of this strcuture of the Coulomb interaction, the effect of screening is different for the singlet and triplet components.

Now we replace $\tilde{\Pi}$ by the RPA polarization function, which is given by[36]

$$\tilde{\Pi}^{(0)}_{\mathrm{ret}m_1m_1',m_2m_2'}(\mathbf{r}_1,\mathbf{r}_2,\omega) = \tilde{\Pi}^{(0)}_{\mathrm{ret}\,m_1m_2}(\mathbf{r}_1,\mathbf{r}_2,\omega)\delta_{m_1m_2'}\delta_{m_2m_1'},$$

$$\tilde{\Pi}^{(0)}_{\mathrm{ret}\,m_1m_2}(\mathbf{r}_1,\mathbf{r}_2,\omega) = -\sum_{\mu\mu'} \frac{f_{\mu m_1} - f_{\mu' m_2}}{E_{\mu' m_2} - E_{\mu m_1} - \hbar(\omega + i\epsilon)} \tilde{\varphi}^*_{\mu}(\mathbf{r}_1)\tilde{\varphi}_{\mu'}(\mathbf{r}_1) \times \tilde{\varphi}^*_{\mu'}(\mathbf{r}_2)\tilde{\varphi}_{\mu}(\mathbf{r}_2). \tag{69}$$

In the coordinates α, β, the matrix of $\tilde{\Pi}^{(0)}$ has the form

$$\tilde{\Pi}^{(0)} = \begin{pmatrix} \tilde{\Pi}^{(0)}_{00} & 0 & 0 & \tilde{\Pi}^{(0)}_{0z} \\ 0 & \tilde{\Pi}^{(0)}_{xx} & 0 & 0 \\ 0 & 0 & \tilde{\Pi}^{(0)}_{yy} & 0 \\ \tilde{\Pi}^{(0)}_{z0} & 0 & 0 & \tilde{\Pi}^{(0)}_{zz} \end{pmatrix}; \quad \begin{matrix} \tilde{\Pi}^{(0)}_{xx} = \tilde{\Pi}^{(0)}_{yy} \\ \tilde{\Pi}^{(0)}_{zz} = \tilde{\Pi}^{(0)}_{00} \\ \tilde{\Pi}^{(0)}_{z0} = \tilde{\Pi}^{(0)}_{0z} \end{matrix}. \tag{70}$$

This structure results from rotational invariance in the spin space and is found also for the exact polarization function $\tilde{\Pi}$. Equation (67) can now easily be solved. We introduce a screened potential $\tilde{V}^{(s)}$[35] with the only nonvanishing components

$$\tilde{V}^{(s)}_{\mathrm{ret}\,00}(\mathbf{q},\omega) = \tilde{v}_{00}(\mathbf{q})\sum_{k=0}^{\infty}[\tilde{L}_{\mathrm{ret}\,00}(\mathbf{q},\omega)\tilde{v}_{00}(\mathbf{q})]^k = \frac{\tilde{v}_{00}(\mathbf{q})}{1-\tilde{\Pi}^{(0)}_{\mathrm{ret}\,00}(\mathbf{q},\omega)\tilde{v}_{00}(\mathbf{q})}. \tag{71}$$

The denominator in Eq. (71) yields the Lindhard dielectric function. With the above definition we obtain a closed expression for the density correlation function

$$\tilde{L}_{\mathrm{ret}\,zz}(\mathbf{q},\omega) = \tilde{\Pi}^{(0)}_{\mathrm{ret}\,zz}(\mathbf{q},\omega) + \tilde{\Pi}^{(0)}_{\mathrm{ret}\,z0} \times (\mathbf{q},\omega)\tilde{V}^{(s)}_{\mathrm{ret}\,00}(\mathbf{q},\omega)\tilde{\Pi}^{(0)}_{\mathrm{ret}\,0z}(\mathbf{q},\omega). \tag{72}$$

For the calculation of the magnetization in mean-field approximation we only need the function $\tilde{L}$ at $\mathbf{q}=0$ and $\omega=0$. Taking into account the spatial homogeneity and employing the orthonormality of the eigenfunctions (69), we obtain

$$\begin{aligned}\tilde{\Pi}^{(0)}_{\mathrm{ret}\,zz}(\mathbf{q}=0,\omega=0) &= \frac{1}{\Omega}\int d^3\mathbf{r}_1 \int d^3\mathbf{r}_2 \tilde{\Pi}^{(0)}_{\mathrm{ret}\,zz}(\mathbf{r}_1,\mathbf{r}_2,\omega) \\ &= \frac{1}{\Omega}\sum_{\mu}\left[\left.\frac{-df(E)}{dE}\right|_{E=E_{\mu\uparrow}} + \left.\frac{-df(E)}{dE}\right|_{E=E_{\mu\downarrow}}\right] \\ &= -\frac{1}{2}[D_{\uparrow}(E_F) + D_{\downarrow}(E_F)] \\ &= -\frac{1}{2}D(E_F),\end{aligned} \tag{73}$$

where Ω_0 is the normalization volume, which is considered in the limit $\Omega\to\infty$ and we assumed $T=0$ so that $-df/dE = \delta(E-E_F)$. The functions $D_{\uparrow}$ and $D_{\downarrow}$ denote the density of states of the electrons in the spin-up and spin-down subbands. Here, we clearly see that the influence of the Landau quantization and the finite temperature is negligible in the limit $\hbar\omega_c \ll k_BT \ll \mu$, where μ is the chemical potential. The relation (73) also follows from the explicit expressions of the range functions. Analogously, for the nondiagonal element of $\tilde{\Pi}^{(0)}$ we find

$$\tilde{\Pi}^{(0)}_{\mathrm{ret}\,z0}(\mathbf{q}=0,\omega=0) = -\tfrac{1}{2}[D_{\uparrow}(E_F) - D_{\downarrow}(E_F)]. \tag{74}$$

Inserting these expressions into Eqs. (71) and (72), we obtain the final result

$$F_{zz}(0) = I^2\frac{D_{\uparrow}(E_F)D_{\downarrow}(E_F)}{D_{\uparrow}(E_F)+D_{\downarrow}(E_F)} = \frac{I^2}{4}[D_{\uparrow}(E_F)+D_{\downarrow}(E_F)]\left\{1-\left[\frac{D_{\uparrow}(E_F)-D_{\downarrow}(E_F)}{D_{\uparrow}(E_F)+D_{\downarrow}(E_F)}\right]^2\right\}. \tag{75}$$

The effect of screening leads to the additional factor in curly brackets, which is equal to unity if $D_{\uparrow}(E_F)=D_{\downarrow}(E_F)$, but vanishes if $D_{\uparrow}(E_F)=0$ or $D_{\downarrow}(E_F)=0$. Because the Zeeman splitting in DMS is not small, the influence of screening is significant. This contribution is also important to establish the equivalence between RKKY theory and mean-field Zener theory.

As discussed in the beginning of this subsection, the magnetic susceptibility (10) does not establish a relationship between M and H, but between dM and dH. For the problem under consideration this means that the relation (61) has to be replaced by the differential equation

$$\left(\frac{\partial B_{\mathrm{exc}}}{\partial M}\right)_{\varrho} = \left(\frac{\partial B_{\mathrm{exc}}}{\partial M}\right)_{E_F} - \left(\frac{\partial B_{\mathrm{exc}}}{\partial E_F}\right)_M \frac{\left(\frac{\partial \varrho}{\partial M}\right)_{E_F}}{\left(\frac{\partial \varrho}{\partial E_F}\right)_M} = \frac{1}{\mu_0}\left(\frac{2m_0}{g_{\mathrm{ion}}e}\right)^2 F_{zz}(0)$$

and the solution is

$$B_{\mathrm{exc}} = \frac{2m_0}{g_{\mathrm{ion}}e}\frac{I}{2}(\varrho_\downarrow - \varrho_\uparrow), \quad \varrho_m = \int_{-\infty}^{E_F} dE D_m(E). \tag{76}$$

This is exactly the expression for the exchange field used in mean-field Zener theory.[3,5]

The Curie temperature for mean-field Zener theory is the same as for the linear theory, Eq. (62), because it is determined by the behavior for small M. With $\varrho_\uparrow = \varrho_\downarrow = \frac{1}{2}\varrho$, we find

$$T_C = \frac{S(S+1)}{3^{2/3}4\pi^{4/3}k_B}\frac{x}{\Omega_0}I^2 m * \varrho^{1/3}. \tag{77}$$

So far, we did not consider the effect of Coulomb interaction on the polarization function. In the generalized random-phase approximation (GRPA), this effect of the approximated as a prefactor $\tilde{\Pi}_{\mathrm{ret}}(\mathbf{q},\omega=0) = \tilde{\Pi}^{(0)}_{\mathrm{ret}}(\mathbf{q},\omega=0)/[1 + \bar{v}(\mathbf{q})\tilde{\Pi}^{(0)}_{\mathrm{ret}}(\mathbf{q},\omega=0)]$, where $\bar{v}(\mathbf{q}) \geqslant 0$ is a parameter for the effective pair interaction.[29,30,52] Then the density of states $D_m(E)$ in Eq. (76) has to be replaced by $D_m(E)/[1 - \bar{v}(0)D_m(E)]$.

The presence of disorder results in an exponential damping of the RKKY interaction due to the finite mean free path.[53–55] It also leads to an effective electron-electron interaction so that the ensemble-averaged function $\langle\langle\tilde{\Pi}^{(0)}\rangle\rangle$ is a sum of ladder-bubble diagrams like in the GRPA.[56] The net effect of disorder is an increase of the RKKY interaction and a reduction of T_C.[3]

VI. SUMMARY AND CONCLUSIONS

In this paper we derived the RKKY interaction in semiconductors, including band degeneracy, modulations of the band edges, and external fields. The function Φ, which determines the coupling, can be traced back to the eigenvalues and eigenfunctions of an effective-mass Hamiltonian, acting in the space of the envelope functions, while the lattice-periodic parts enter the effective Hamiltonian only through matrix elements, which, up to prefactors, follow from crystal symmetry.

We presented analytical results for the range function of a three- and two-dimensional semiconductor in a magnetic field. In the limit of vanishing field, we recover the well-known range functions F_3 and F_2, respectively. We also gave an explicit expression in the limit of large magnetic field, in the case that only one Landau level is occupied.

If Zeeman splitting of the bands is taken into account, the RKKY Hamiltonian is no longer isotropic. For the Γ_6 conduction band under consideration and $\mathbf{B}_{\mathrm{ext}} \| \mathbf{e}_z$, it is found that the RKKY interaction has two principal axes with $\Phi_{xx} = \Phi_{yy} \neq \Phi_{zz}$.

In the presence of Zeeman splitting, the RKKY interaction is significantly changed due to screening on the account of electron-electron interaction. In particular, $F_{zz}(0)$ becomes zero if one subband edge lies above the Fermi level. It is rigorously shown that the RKKY result, including screening, is equivalent to mean-field Zener theory.

A critical point of the theory so far is the introduction of a magnetic Hamiltonian through the VCA. In reality, the magnetic impurities should lead to bound states and to a localization of the eigenfunctions, especially in the limit $\rho \ll x/\Omega_0$. A recent study based upon Monte Carlo calculations revealed significant derivation from the mean-field-VCA results, which were addressed to short-range magnetic order and local carrier spin polarization.[4] There is much current interest in understanding the role of bound magnetic polarons for the formation of ferromagnetism in DMS.[57–59] These topics will be the subject of further studies.

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