30, 227 (1973).
[10]Ya. Pokrovskiĭ, Phys. Status Solidi [a] 11, 385 (1972).
[11]T. K. Lo, B. J. Feldman, and C. D. Jeffries, Phys. Rev. Lett. 31, 224 (1973).
[12]J. C. McGroddy, M. Voos, and O. Christensen, Solid State Commun. 13, 1801 (1973).
[13]V. A. Shcherbov, E. M. Kuleshov, and A. N. Goroshko, Voprosy radioelecktroniki, seriya Radioizmeritel'naya tekhnika 9, (1970).
[14]E. H. Putley, Phys. Status Solidi 6, 571 (1964).
[15]K. Muro and J. Nisida, Solid State Commun. 15, 1663 (1974).
[16]A. Frova, G. A. Thomas, R. E. Miller, and E. O. Kane, Preprint Bell Labor., No. 07974, New Jersey, 1974.
[17]R. Barrie and K. Nishikawa, Can. J. Phys. 41, 1823 (1963).
[18]L. V. Keldysh, in: Eksitony v poluprovodnikakh (Excitons in Semiconductors), No. 5, Nauka, 1971.
[19]Ya. E. Pokrovskiĭ and K. I. Svistunova, Pis'ma Zh. Eksp. Teor. Fiz. 13, 297 (1971) [JETP Lett. 13, 212 (1971)].
[20]V. S. Bagaev, N. A. Penin, N. N. Sibel'din, and V. A. Tsvetkov, Fiz. Tverd. Tela 15, 3269 (1973) [Sov. Phys. Solid State 15, 2179 (1974)].
[21]V. S. Bagaev, N. V. Zamkovets, L. V. Keldysh, N. N. Sibel'din, and V. A. Tsvetkov, Preprint FIAN, Moscow, 1975.
[22]A. S. Alekseev, T. A. Astemirov, V. S. Bagaev, T. I. Galkina, N. A. Penin, N. N. Sibel'din, and V. A. Tsvetkov, Proc. Twelfth Intern. Conf. on Physics of Semiconductors, Stuttgart, 1974.
[23]V. S. Bagaev, N. N. Sibel'din, and V. A. Tsvetkov, Pis'ma Zh. Eksp. Teor. Fiz. 21, 180 (1975) [JETP Lett. 21, 80 (1975)].

Translated by J. G. Adashko

A possible resonance method for investigating electron-impurity exchange interaction in semiconductors

S. K. Savvinykh

Institute of Semiconductor Physics, Siberian Division, USSR Academy of Sciences, Novosibirsk

(Submitted August 4, 1975)
Zh. Eksp. Teor. Fiz. 70, 235–240 (January 1976)

An analysis is made of carrier states localized on a paramagnetic impurity in a nondegenerate semiconductor subjected to crossed magnetic and electric fields. It is shown that the exchange part of the electron-impurity interaction, which couples the orbital and spin coordinates of an electron, may give rise to electric-dipole transitions between the electron-impurity multiplet states. The probabilities of these transitions are calculated and found to be several orders of magnitude higher than the probabilities of magnetic-dipole transitions.

PACS numbers: 71.70.Gm, 71.55.—i

I. INTRODUCTION

In a static magnetic field a potential well, no matter how shallow, creates a localized state with the binding energy[1,2]

$$\varepsilon_b \propto \Omega (a/l)^2, \tag{1}$$

where Ω is the cyclotron frequency, $l=(c/eH)^{1/2}$ is the magnetic length, and a is the scattering length of an electron interacting with a potential center in the absence of a magnetic field ($\hbar=1$). We shall show later that a similar situation arises when an impurity center has spin (paramagnetic impurity). In this case the energy spectrum of localized states created by a magnetic field has a characteristic structure of an electron—impurity spin multiplet.

We shall show that in addition to the usual magnetic-dipole transitions between the states of this multiplet, which can be investigated by the ESR methods, there may be also transitions of the electric-dipole type whose intensities are several orders of magnitude higher than those of magnetic-dipole transitions. The separation between the energy levels of a multiplet and the transition probabilities are functions of the parameters of the electron—impurity exchange and it is natural to expect that these parameters may be determined most conveniently using electric-dipole resonant transitions.

The interaction between a paramagnetic impurity center, whose spin is S, and a free carrier (electron) can be described by the model Hamiltonian

$$\mathscr{H}_{\rm int}=V(r)+J(r)\,\mathbf{S}\cdot\mathbf{s}. \tag{2}$$

We shall assume that a paramagnetic center has a spin $S=\frac{1}{2}$. Moreover, we shall postulate that the interaction (2) corresponds to attraction in both spin states (singlet and triplet) of the electron—impurity system.

We shall be interested primarily in the case when the electron—impurity interaction results in localization of an electron only in the presence of a magnetic field. The resultant localized states are characterized by a low binding energy ($\varepsilon_b \to 0$ for $H\to 0$) and large spatial dimensions, given by the quantity l at right-angles to the magnetic field and by $(2m\varepsilon_b)^{-1/2}$ along the field. Therefore, states of this kind can be described by the approximation of "zero-radius" potential, which improves in precision with decreasing H. In this approximation the interaction Hamiltonian (2) is governed entirely by two scattering lengths: a_t and a_s, corresponding to the triplet and singlet spin states of the electron—impurity system. In this model, the main contribution of the exchange forces is given by

$\tilde{\gamma}=(a_t-a_s)/(a_t+a_s)$.

An important feature of our discussion is that the Hamiltonian (2) couples ("mixes") the coordinate and spin variables. The second term in Eq. (2) represents the spin–orbit interaction due to exchange. This spin–orbit coupling, which does not have a relativistic small term, is the main cause of the appearance of electric-dipole transitions between the electron–impurity multiplet states which are characterized by zero projection of spin along the magnetic field.

However, the spin–orbit coupling is a necessary but not a sufficient condition for the appearance of electric-dipole transitions in the problem under discussion. The dipole moment of the localized states and its matrix elements, governing the transition probabilities, all vanish because of the radial symmetry of the wave functions in the plane perpendicular to the magnetic field. Therefore, we shall assume that, in addition to a static magnetic field, a crystal is subjected to a static electric field E, which is normal to the magnetic field. The electric field distorts the radial symmetry of the wave functions and a measure of distortion of these functions is $\gamma=eEl/\Omega$. Under these conditions the probability of electric-dipole transitions W_E is no longer zero. We can show that the ratio of this probability to the probability of allowed magnetic-dipole transitions is

$$W_E/W_M\sim(\gamma\tilde{\gamma})^2(l/\lambda\!\!\!^-)^2, \tag{3}$$

where $\lambda\!\!\!^-$ is the Compton wavelength of an electron. The factor $(l/\lambda\!\!\!^-)^2$ makes the ratio W_E/W_M usually very large, in spite of the fact of the smallness of γ and possible smallness of $\tilde{\gamma}$ assumed in later calculations.

The rest of our discussion will apply to the case of a nondegenerate electron gas with an isotropic quadratic dispersion law (the model of a single-band nondegenerate semiconductor). The absence of degeneracy allows us to consider the interaction of an electron with a paramagnetic impurity in the single-particle framework.

2. ENERGY SPECTRUM AND WAVE FUNCTIONS OF LOCALIZED STATES

The energy levels and wave functions of localized states will be found using the results of [3] where the electron scattering operator in the presence of a static magnetic field is found for the interaction (2). The relationships derived there can be generalized in a self-evident manner to the case of crossed electric and magnetic fields: $\mathbf{H}=(0,0,H)$, $\mathbf{E}=(E,0,0)$. In the expression

$$K(\varepsilon)=\frac{2\pi i}{m}\frac{\partial rG_0(r,0)}{\partial r}\Big|_{r=0}$$

it is sufficient to regard G_0 as the Green function in crossed fields. The function $K(\varepsilon)$ found in[4] is then of the form

$$K(\varepsilon)=\frac{1}{4l}\left(\frac{2i}{\pi}\right)^{1/2}\int_0^\infty\frac{dt}{t^{1/2}}\left\{\frac{2}{t}-\frac{\exp[i(\varepsilon/\Omega-\gamma^2/2)t+{}^1/_4 i\gamma^2t^2\operatorname{ctg}(t/2)]}{\sin(t/2)}\right\}. \tag{4}$$

We shall be interested only in the states whose total-spin projection on the z axis is zero. The energy levels of these states, governed by the positions of the scattering operator poles, can be found[3] from the expression

$$\left[1+iaK\left(\varepsilon+\frac{\omega_e-\omega_i}{2}\right)\right]\left[1+iaK\left(\varepsilon-\frac{\omega_e-\omega_i}{2}\right)\right]+\tilde{\gamma}^2a^2K\left(\varepsilon+\frac{\omega_e-\omega_i}{2}\right)K\left(\varepsilon-\frac{\omega_e-\omega_i}{2}\right)=0, \tag{5}$$

where $\omega_{e,i}=g_{e,i}\beta H$ are the values of the splitting of spin levels of the electron and the impurity, respectively.

When the exchange part of the interaction vanishes ($\tilde{\gamma}=0$), Eq. (5) reduces to the equation for the spinless problem, analyzed by Drukarev and Monozon. [5] It seems that the results obtained by them would require refinement in respect of the stationary states (Sec. 3).

In calculating the integral in Eq. (4) for $\gamma\ll 1$ it is convenient to direct the integration path along a line rotated into the lower half-plane by an angle θ, where $-\pi/4<\theta<0$. This makes it possible to expand the exponential function in the integrand in terms of $\gamma^2t^2[i\operatorname{ctg}\times(t/2)+1]$. Retaining the first two terms of the expansion, we can transform Eq. (4) to

$$K(\varepsilon)=-\frac{i}{2^{1/2}l}\left\{\zeta\left(\frac{1}{2},x\right)-x^{-1/2}+\frac{3\gamma^2}{16}\left[2\zeta\left(\frac{3}{2},x\right)+(1-2x)\zeta\left(\frac{5}{2},x\right)-x^{-5/2}\right]+\frac{\sqrt{2i}}{(2\gamma^2)^{1/4}}\exp\left(-\frac{x^2}{2\gamma^2}\right)D_{-1/2}\left(\frac{i\sqrt{2}x}{\gamma}\right)\right\}, \tag{6}$$

where $\zeta(p/2,x)$ is a generalized zeta function, $D_{-1/2}(x)$ is a parabolic cylindrical function, and $x=\frac{1}{2}-(\varepsilon/\Omega-\gamma^2/2)$. Subject to an additional assumption $|\gamma/x|\ll 1$, Eq. (6) becomes

$$K(\varepsilon)=-\frac{i}{2^{1/2}l}\left\{\zeta\left(\frac{1}{2},x\right)+\frac{i\sqrt{2}}{x^{1/2}}\exp\left(-\frac{x^2}{\gamma^2}\right)+\frac{3\gamma^2}{16}\left[2\zeta\left(\frac{3}{2},x\right)+(1-2x)\zeta\left(\frac{5}{2},x\right)\right]\right\}, \tag{7}$$

which corresponds to the Drukarev and Monozon result[5] apart from the exponential term which is absent from their expression and which is responsible for the decay of localized states. The decay is a natural manifestation of the fact that an energy level appears against the background of a continuous spectrum.

In the next section we shall calculate the probability of an electric-dipole transition in the specific case when a static electric field is sufficiently weak and we shall ignore its influence on the energy spectrum of localized states but allow for its influence on the wave functions. Therefore, we shall now assume

$$K(\varepsilon)=-i\zeta({}^1/_2,x)/\sqrt{2}l. \tag{8}$$

Omitting analysis of Eq. (5), which is fully analogous to that given by Demkov and Drukarev, [2] we shall quote the final expressions for the energy levels on the assumption that the magnetic field is sufficiently weak:

$$|A|=|a/\sqrt{2}l|\ll 1,\quad a={}^1/_2(a_t+a_s).$$

We shall consider two cases:

1. $a<0$, $\tilde{\gamma}^2\lesssim 1$,

$$\varepsilon_{1,2}\approx\Omega\left(\frac{1}{2}\mp\Delta\right)-\frac{e^2H^2a^2}{2mc^2}\left[1+2|A|\left(\zeta\left(\frac{1}{2}\right)+\tilde{\gamma}^2\zeta\left(\frac{1}{2},\pm2\Delta\right)\right)\right], \tag{9}$$

where $\Delta = (\omega_e - \omega_i)/2\Omega$;

2. $a > 0,\ \tilde{\gamma}^2 \lesssim 1$,

$$\varepsilon_{1,2} \approx -\frac{1}{2ma_{t,s}^2} + \frac{e^2 a_{t,s}^2 H^2}{2mc^2}\left[\frac{1}{12} - \frac{\Delta^2}{\tilde{\gamma}}(2\tilde{\gamma} \mp 1)\right]. \tag{10}$$

The formula (10) represents localized states with a low binding energy which may exist even in the absence of a magnetic field.

We shall conclude this section by giving the expressions for the wave functions of localized states which—in accordance to the well-known rules[6]—can be found from the scattering operator[3]:

$$\Psi_{1,2}(\alpha) = \left(-\frac{2\pi\sqrt{2}\, l\Omega}{mD'(x_{1,2})}\right)^{1/2}\left\{\frac{F^{1/2}(x_{1,2}-\Delta)}{\varepsilon_{1,2}-\varepsilon_{\alpha,+}}\xi_{(+-)} + \frac{F^{1/2}(x_{1,2}+\Delta)}{\varepsilon_{1,2}-\varepsilon_{\alpha,-}}\xi_{(-+)}\right\}, \tag{11}$$

where

$$\alpha = (n, k_y, k_z),\quad \varepsilon_{\alpha,\pm} = \varepsilon_\alpha \pm \Delta\Omega,$$
$$\varepsilon_\alpha = \Omega(n + {}^1/_2) - eEk_y l^2 + k_z^2/2m,$$
$$F(x) = 1 + (1 - \tilde{\gamma}^2)A\zeta({}^1/_2, x),$$
$$D'(x) = A[\zeta'({}^1/_2, x+\Delta)F(x-\Delta) + \zeta'({}^1/_2, x-\Delta)F(x+\Delta)],$$

$\xi_{(+-)}$ and $\xi_{(-+)}$ are the basis unit vectors in the spin space corresponding to zero projections of the total spin on the z axis, and $\varphi_\alpha(0)$ is the wave function of a free electron in crossed electric and magnetic fields at the point of location of an impurity.

3. PROBABILITY OF ELECTRIC-DIPOLE TRANSITIONS

We shall consider transitions between states Ψ_1 and Ψ_2 under the action of an electric field $\tilde{E}$ of frequency ω polarized in the xy plane. In the Landau representation, the electric-dipole interaction operator is of the form

$$\tilde{\mathscr{H}}_{\alpha\alpha'} = \frac{ie}{\omega}\left(\frac{\Omega}{m}\right)^{1/2}\delta_{k_y k_y'}\delta_{k_z k_z'}(n^{1/2}\delta_{n-1,n'}\tilde{E}_- - (n+1)^{1/2}\delta_{n+1,n'}\tilde{E}_+), \tag{12}$$

where

$$\tilde{E}_\pm = (\tilde{E}_x \pm i\tilde{E}_y)/\sqrt{2}.$$

We shall assume that the alternating electric field is sufficiently weak and, therefore, the problem of finding the transition probability reduces—as usual—to the calculation of the matrix element $(\Psi_1 \tilde{\mathscr{H}} \Psi_2)$. Omitting simple but fairly tedious transformations, in which only the main terms containing the small parameter γ are retained, we find that Eqs. (11) and (12) give

$$(\Psi_1\tilde{\mathscr{H}}\Psi_2) = \frac{iae}{4m\omega l^3}\left(\frac{\Omega}{m}\right)^{1/2}\frac{\gamma\tilde{\gamma}}{[F_1^{(-)}F_2^{(+)}D'(x_1)D'(x_2)]^{1/2}}$$
$$\times\left\{\frac{F_1^{(-)}\Phi_+(x_1,x_2) + F_2^{(+)}\Phi_-(x_1,x_2)}{\varepsilon_2-\varepsilon_1+\Omega}\tilde{E}_- + \frac{F_1^{(-)}\Phi_+(x_2,x_1) + F_2^{(+)}\Phi_-(x_2,x_1)}{\varepsilon_2-\varepsilon_1-\Omega}\tilde{E}_+\right\}, \tag{13}$$

where

$$\left.\begin{aligned} &F_{1,2}^{(\pm)} \equiv F(x_{1,2}\pm\Delta),\\ &\Phi_\pm(x_1,x_2) = \sum_{n=1}^{\infty}\left(\frac{n+1}{(n+x_1\pm\Delta)^{3/2}} - \frac{n+1}{(n+x_2\pm\Delta-1)^{3/2}}\right). \end{aligned}\right\} \tag{14}$$

In the calculations based on Eqs. (13) and (14) we shall assume that the magnetic field is sufficiently weak ($|A| \ll 1$) and we shall retain only the principal terms with the small parameter A. Then, in the case when localized states appear only in the presence of an external magnetic field ($a < 0,\ \tilde{\gamma}^2 < 1$), we find that the matrix element is

$$(\Psi_1\tilde{\mathscr{H}}\Psi_2)^{(1)} = \frac{i\sqrt{2}\,e}{m\omega l^2}\left(\frac{\Omega}{m}\right)^{1/2}\gamma\tilde{\gamma}\left(\frac{\tilde{E}_-}{\varepsilon_2-\varepsilon_1+\Omega} + \frac{\tilde{E}_+}{\varepsilon_2-\varepsilon_1-\Omega}\right). \tag{15}$$

If states localized at a paramagnetic impurity exist also in the absence of a magnetic field ($a > 0,\ \tilde{\gamma}^2 < 1$), calculations based on Eq. (13) reduce to

$$(\Psi_1\tilde{\mathscr{H}}\Psi_2)^{(2)}$$
$$= \frac{i\sqrt{2}eA^2\Delta}{m\omega l^2}\frac{\gamma\tilde{\gamma}}{(1-\tilde{\gamma}^2)^{1/2}}\left(\frac{\Omega}{m}\right)^{1/2}\left[\frac{(1+\tilde{\gamma})(1+3\tilde{\gamma})}{\varepsilon_2-\varepsilon_1-\Omega}\tilde{E}_- - \frac{(1-\tilde{\gamma})(1-3\tilde{\gamma})}{\varepsilon_2-\varepsilon_1+\Omega}\tilde{E}_+\right]. \tag{16}$$

In this case the probability of an electric-dipole transition is considerably lower:

$$\frac{W_E^{(2)}}{W_E^{(1)}} = \frac{|(\Psi_1\tilde{\mathscr{H}}\Psi_2)^{(2)}|^2}{|(\Psi_1\tilde{\mathscr{H}}\Psi_2)^{(1)}|^2} \sim A^8 \ll 1.$$

The validity of Eqs. (15) and (16) is governed by the inequalities $l \gg a,\ \gamma = eEl/\Omega \ll 1$, which—for $a = 10^{-7}$ cm, $m \approx m_0 \approx 10^{-27}$ g, and $E \approx 1$ V/cm—are equivalent to the condition $10^3\ G \ll H \ll 10^7$ G.

4. CONCLUSIONS

The interaction of carriers with paramagnetic impurities, which gives rise to several fine physical effects, has for long been an important subject in the physics of metals and semiconductors. In the majority of investigations this interaction is the cause of carrier scattering which to a greater or smaller extent governs the equilibrium and transport properties of a solid. It is natural to expect also the properties of a paramagnetic impurity and the nature of its interaction with free carriers to be manifested most clearly and directly in the structure of the spectrum and wave functions of bound states when a paramagnetic impurity becomes a localization center of a carrier. In this connection we may hope that a resonance involving electric-dipole transitions between states of the type discussed above will serve as a basis for a method of detection of paramagnetic impurities and investigation of their interaction with carriers in semiconductor crystals.

[1]Yu. A. Bychkov and A. M. Dykhne, Zh. Eksp. Teor. Fiz. 48, 1174 (1965) [Sov. Phys.-JETP 21, 783 (1965)].

[2]Yu. N. Demkov and G. F. Drukarev, Zh. Eksp. Teor. Fiz. 49, 257 (1965) [Sov. Phys.-JETP 22, 182 (1966)].

[3]S. K. Savvinykh, Fiz. Tverd. Tela (Leningrad) 16, 490 (1974) [Sov. Phys.-Solid State 16, 313 (1974)].

[4]L. I. Magarill and S. K. Savvinykh, Zh. Eksp. Teor. Fiz. 60, 175 (1971) [Sov. Phys.-JETP 33, 97 (1971)].

[5]G. F. Drukarev and B. S. Monozon, Zh. Eksp. Teor. Fiz. 61, 956 (1971) [Sov. Phys.-JETP 34, 509 (1972)].

[6]A. I. Baz', Ya. B. Zel'dovich, and A. M. Perelomov, Rasseyanie, reaktsii i raspady v nerelyativistskoi kvantovoi mekhanike, Nauka, M., 1971 (Scattering, Reactions and Decay in Nonrelativistic Quantum Mechanics, Israel Program for Scientific Translations, Jerusalem, 1969).

Translated by A. Tybulewicz