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Configuration interaction in delta-doped heterostructures

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We analyze the tunnel coupling between an impurity state located in a δ-layer and the 2D delocalized states in the quantum well (QW) located at a few nanometers from the δ-layer. The problem is formulated in terms of Anderson–Fano model as configuration interaction between the carrier bound state at the impurity and the continuum of delocalized states in the QW. An effect of this interaction on the interband optical transitions in the QW is analyzed. The results are discussed regarding the series of experiments on the GaAs structures with a δ-Mn layer.

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1. Introduction

The problem of so-called configuration interaction of a single bound state with a continuum of states goes back to the famous paper by U. Fano [1] rated as one of the most relevant works of 20th century [2]. The suggested theoretical approach often regarded as Fano–Anderson model or configuration interaction succeeded in explaining puzzling asymmetric resonances observed in various experiments in atomic and nuclear physics, condensed matter physics and optics [2]. The co-existence of the discrete energy level and the continuum states within the same energy range is also quite common in low-dimensional semiconductor structures [2–5]. Of particular interest nowadays are the structures having a quantum well (QW) and a ferromagnetic or paramagnetic layer located in the vicinity of the QW, but not penetrating into the QW region. In such structures high mobility of the carriers along the QW is combined with the magnetic properties provided by the magnetic layer. A number of recent experiments show that the Mn δ-layer gives rise to circular polarization of the photoluminescence (PL) from the QW in an external magnetic field applied perpendicular to the QW plane [6,7]. It was questioned whether the spin polarization of the carries in the QW is due to the electrons tunneling to Mn site or the tunnel coupling of the holes at Mn with those in the QW. The latter mechanism seemed to lack the proper theoretical description. In this paper we try to fill this gap. We show that the simple scheme of the holes configuration interaction leads to the opposite sign of the circular polarization than that observed in the experiment. The model system considered in the present paper consists of a δ-layer of the impurities (donors or acceptors) and a QW having one level of size quantization for the electrons or holes, respectively. The energy level of the impurity bound state lies within the range of the 2D states size quantization subband in the QW. We will be considering the case of rather deep impurity level in the sense that the impurity activation energy substantially exceeds the kinetic energy of the 2D carriers in the QW. The attracting potential of the impurity is assumed spherically symmetric and since it is a deep level we treat it with zero radius potential approximation [8]. At that we consider both the simple band structure and the one of the GaAs valence band type.

2. Tunneling between impurity and quantum well

In this section we consider the configuration interaction between a single impurity bound state and the continuum of 2D states in the QW. The potential barrier separating the impurity from the QW is assumed to be weakly transparent for the tunneling. Rigorous calculation of the eigenfunctions is rather hard to perform as it requires solving stationary Schrödinger equation in the complicated 3D potential. In order to circumvent the explicit solving of the Schrödinger equation for tunneling problems the so-called tunneling or transfer Hamiltonian formalism is commonly used as originally proposed by Bardeen [9]. The total Hamiltonian

is expressed as $H = H_i + H_{QW} + H_T$, where H_i is partial Hamiltonian having the bound state at the impurity as its eigen state. H_{QW} in the same way corresponds to the QW itself, its eigenfunctions φ_λ form nondegenerate continuum of states characterized by the quantum number(s) λ. The term H_T accounts for the tunneling. In the secondary quantization representation the total Hamiltonian can be written as follows:

$$H = \varepsilon_0 a^+ a + \int \varepsilon_\lambda c_\lambda^+ c_\lambda d\lambda + \int (t_\lambda c_\lambda^+ a + t_\lambda^* a^+ c_\lambda) d\lambda, \quad (1)$$

where a^+, a are the creation and annihilation operators for the bound state characterized by its energy ε_0, and c_λ^+, c_λ are the creation and annihilation operators for a continuum state having energy ε_λ. The energy here and below is measured from the level of size quantization of the carriers in the QW so that ε_λ is simply their kinetic energy. The expression (1) is rather general, in fact it can be regarded as introducing the coupling between two systems into the Hamiltonian in the most simple phenomenological way. From this viewpoint the coupling parameter t_λ is still to be determined through exact solving of the eigenvalue problem for the whole system. Bardeen's approach suggests a simple recipe for calculation of the tunneling parameter for the case of weak tunneling through a potential barrier:

$$t_\lambda = \int_\Omega (\varphi_\lambda^* K\psi - \psi K\varphi_\lambda^*)\, d\mathbf{r}, \quad (2)$$

where integration is performed over the region Ω to the one side of the barrier. Here K is the kinetic energy operator:

$$K = -\frac{\hbar^2}{2m}\Delta. \quad (3)$$

The attraction potential of the impurity is considered spherically symmetric, so the whole system (impurity+QW) has the cylindrical symmetry with z axis directed normally to the QW plane and going through the impurity center. Thus for further calculations it will be most convenient to represent the QW states in cylindrical coordinates rather than as plane waves. In this case each state is characterized by the wavenumber k and the cylindrical harmonic number l:

$$\varphi_{kl} = \eta(z)\sqrt{\frac{m}{2\pi\hbar^2}} J_l(k\rho)\, e^{il\theta}, \quad (4)$$

where $J_l(k\rho)$ is the Bessel function of order l, ρ and θ are the polar coordinates in the QW plane, m is the in-plane effective mass, $\eta(z)$ is the envelope function of size quantization in z direction. The wavefunction (4) has the normalization:

$$\langle \varphi_{kl} \mid \varphi_{k'l'} \rangle = \delta(\varepsilon - \varepsilon')\delta_{ll'}, \quad (5)$$

where $\varepsilon = \hbar^2 k^2/2m$. The potential barrier separating the deep impurity level from the QW in the first approximation can be assumed having a rectangular shape. Inside the barrier the function $\eta(z)$ is (z axis is directed towards the impurity, $z = 0$ corresponds to the QW boundary)

$$\eta(z) \sim \frac{1}{\sqrt{a}} e^{-qz}, \quad (6)$$

where $q = \sqrt{2mE_0/\hbar^2}$, a is the QW width, E_0 is the binding energy of the bound state, at the same time E_0 determines the height of the potential barrier. Let us firstly consider the simple band case valid for the bound electrons at donor impurity coupled to the QW conductance band. The spherical potential of the impurity results in the ground state of the carrier to be angular independent, therefore the efficient tunneling overlap occurs only with the zeroth cylindrical harmonic $\varphi_{k0} \equiv \varphi(\varepsilon)$. For the deep impurity level one can use zero radius potential approximation [8] and express the *s*-type wavefunction as

$$\psi = \sqrt{2q}\,\frac{e^{-qr}}{r}. \quad (7)$$

The volume integral (2) is reduced to the surface integral over the surface Ω_S inside the barrier which is more convenient to take at the impurity site. This yields for the electrons tunneling between the donor state and the QW:

$$t_k^e = \sqrt{\frac{2\pi}{aq(1+k^2/q^2)}}\sqrt{E_0}\, e^{-qd}. \quad (8)$$

It is clearly seen that as long as the case $k << q$ is considered, the tunneling parameter has very weak dependence on k.

In order to apply the same approach to the holes tunneling in GaAs it has to be generalized for the case of the valence band complex structure. Let us consider $In_xGa_{1-x}As$ QW having only one level of size quantization for the heavy holes and neglect the light holes being split off due to the size quantization. The basis of Bloch amplitudes to be used is formed of the states with certain projection of the total angular momentum $J = 3/2$ on z axis. It would be tempting to generalize (2) by treating K as the kinetic part of the Luttinger Hamiltonian ($\hbar k_x$, $\hbar k_y$, $\hbar k_z$ are, as usual, the momentum operators along the appropriate axis):

$$K = \begin{pmatrix} F & H & I & 0 \\ H^* & G & 0 & I \\ I^* & 0 & G & -H \\ 0 & I^* & -H^* & F \end{pmatrix}, \quad (9)$$

$$F = -Ak^2 - \frac{B}{2}(k^2 - 3k_z^2),$$

$$G = -Ak^2 + \frac{B}{2}(k^2 - 3k_z^2),$$

$$H = Dk_z(k_x - ik_y),$$

$$I = \frac{\sqrt{3}}{2}B(k_x^2 - k_y^2) - iDk_xk_y. \quad (10)$$

The functions ψ_α, $\varphi_{\lambda\beta}$ in (2) become now 4-component vector functions (also the spin indices α and β are added here). The explicit expression for the bound hole state functions ψ_α and the 2D hole states $\varphi_{\lambda\beta}$ can be found in Ref. 10. The important thing about those is while the decay length in z direction of the 2D wavefunctions $\varphi_{\lambda\beta}$ is controlled by the heavy hole mass $m_{hh} \approx 0.5\, m_0$ (m_0 is the free electron mass), the decay length of radial part of the bound state wavefunction ψ_α is characterized by both heavy hole mass m_{hh} and the light hole mass $m_{lh} \approx 0.08\, m_0$ [10]. Analogously to the simple band case the integration (2) over the whole space is reduced to the integration over the surface Ω_S inside the barrier, at that, only z projection of the kinetic energy operator is required. The expression for tunneling parameter simplifies into

$$t_{kl\alpha\beta}^{(h)} = (B-A)\int\limits_{\Omega_S} dS\left(\varphi_{kl\beta}^{*}\frac{d}{dz}\psi_\alpha - \psi_\alpha\frac{d}{dz}\varphi_{kl\beta}^{*}\right), \quad (11)$$

where φ_{kl} is given by (4).

Regrettably, the above given straightforward generalization of (2) fails to be fully correct. Indeed, the largest decay length of the bound state ψ_α is determined by the light hole mass while the decay length of the QW states is governed by the heavy hole. Due to this circumstance the result of the surface integration (11) becomes dependent on the particular position of the integration surface inside the barrier. However, it can be shown that in the case of two different masses the exponential dependence of the tunneling parameter on the barrier thickness is determined by the smallest mass, but the exact value of the tunneling parameter cannot be correctly obtained within the given approach. Now we define $q = \sqrt{2m_{hh}E_0}/\hbar^2$, $\beta = m_{lh}/m_{hh}$. The explicit evaluation of the overlap integrals with account for $k << q$ shows that the tunneling configuration interaction to be accounted for is only between the zeroth cylindrical harmonic $\varphi_{k0,-3/2}$ and the bound state $\psi_{-3/2}$ as well as between $\varphi_{k0,+3/2}$ and $\psi_{+3/2}$. Both are governed by the same tunneling parameter t_k^h:

$$t_k^h = \left(\frac{A-B}{\hbar^2/2m_0}\right)\sqrt{\frac{\pi}{aq}}\sqrt{\frac{m_{hh}m'_{hh}}{m_0^2}}\zeta(k/q)\beta\sqrt{E_0}\times$$

$$\times\exp\left(-\chi(k/q)\sqrt{\beta}qd\right), \quad (12)$$

where $1 \le \chi \le 2$, $\zeta \sim 1$ are weak dimensionless functions of k/q, m'_{hh} is the effective in-plane heavy hole mass. The tunneling parameter t_k^h exponentially depends on the barrier thickness with the light hole mass entering the exponent index. The particular expressions for χ and ζ depend on the surface one chooses for the integration in (2).

In both cases for t_k^e, t_k^h it is reasonable to assume that the tunneling parameter does not depend on k as weak tunneling implies $k << q$. Still, its rapidly decreasing behavior for $k >> q$ has to be kept in mind when it provides convergence for integration over k. In our estimations the shape of the potential barrier separating the QW was assumed rectangular. This is quite reasonable for the estimation at $k << q$. However, the particular shape of the barrier becomes important when one is concerned with experimental dependence on the distance d between the impurity and the QW.

3. Effect on the luminescence spectrum

The transfer Hamiltonian (1) with known tunneling parameter $t(\varepsilon)$ allows one to construct the eigenfunctions Ψ of the whole system given those of the bound state ψ and the QW states $\varphi(\varepsilon)$:

$$\Psi(E) = \nu_0(E)\psi + \int\limits_0^\infty \nu(E,\varepsilon)\varphi(\varepsilon)d\varepsilon, \quad (13)$$

E denotes the energy of the state Ψ. Here $\varphi(\varepsilon)$ are the wavefunctions with zeroth cylindrical harmonic, as was shown above the other harmonics are not affected by the tunneling configuration interaction. Plugging (13) into the stationary Schrödinger equation

$$H\Psi = E\Psi$$

with H being the effective Hamiltonian (1) one gets the following system of equations:

$$\begin{aligned}\nu_0(E)\varepsilon_0 + \int\limits_0^\infty t(\varepsilon)\nu(E,\varepsilon)\,d\varepsilon &= E\nu_0(E),\\ \nu(E,\varepsilon)\varepsilon + t(\varepsilon)\nu_0(E) &= E\nu(E,\varepsilon).\end{aligned} \quad (14)$$

In the present work we consider the case of the bound level energy lying within the range of the continuum: $\varepsilon_0 >> t^2$. For this case the solution is obtained as shown in Ref. 1:

$$\nu_0{}^2(E) = \frac{t^2(E)}{\pi^2 t^4(E) + (E-\tilde{\varepsilon}_0)^2},$$

$$\nu(E,\varepsilon) = \nu_0(E)\left(P\frac{t(\varepsilon)}{E-\varepsilon} + Z(E)t(E)\delta(E-\varepsilon)\right), \quad (15)$$

where

$$Z(E) = \frac{E-\varepsilon_0-F(E)}{t^2(E)},$$

$$F(E) = \int\limits_0^\infty P\frac{t^2(\varepsilon)}{(E-\varepsilon)}d\varepsilon, \quad (16)$$

P stands for the principal value and $\tilde{\varepsilon}_0$ is the center of configuration resonance, which appears to be slightly shifted from ε_0:

$$\tilde{\varepsilon}_0(E) = \varepsilon_0 + F(E). \quad (17)$$

Because of $k << q$ it is reasonable to put $t =$ const everywhere, except for (16) where decrease of t at $E \to \infty$ is necessary for convergence of the integral.

In order to analyze the influence of the configuration interaction on the luminescence spectra we have to calculate matrix element of operator $\hat{M}$ describing interband radiative transitions between the hybridized wavefunction $\Psi(E)$ and wavefunction of 2D the carrier in the other band of the QW which we denote by $\xi_{k'l'}$, here k' is the magnitude of the wavevector, l' is the number of cylindrical harmonic analogously to (4). If, for instance, one considers the acceptor-type impurity then $\Psi(E)$ is the hybridized wavefunction of the 2D holes and $\xi_{k'l'}$ is the wavefunction of the 2D electrons in the QW. We assume that (a) there are no radiative transitions between the bound state wavefunction ψ and the 2D carrier wavefunction $\xi_{k'l'}$ in the other band thus the matrix element for transitions from the bound state:

$$\left\langle \xi_{k'l'} \left| \hat{M} \right| \psi \right\rangle = 0, \tag{18}$$

(b) the interband radiative transitions between the free 2D states in the QW are direct. According to (4) the wavefunctions $\varphi(\varepsilon)$ and $\xi(\varepsilon')$ corresponding to the zeroth harmonic in the cylindrical basis are

$$\varphi(\varepsilon) = \eta(z)\sqrt{\frac{m}{2\pi\hbar^2}}J_0(k\rho),$$

$$\xi(\varepsilon') = \zeta(z)\sqrt{\frac{m'}{2\pi\hbar^2}}J_0(k'\rho), \tag{19}$$

where

$$k = \frac{\sqrt{2m\varepsilon}}{\hbar}, \qquad k' = \frac{\sqrt{2m'\varepsilon'}}{\hbar},$$

$\eta(z), \zeta(z)$ are the appropriate size quantization functions in z direction, m, m' are the in-plane masses of the electrons and holes, respectively, if the donor-type impurity is considered and vice versa for the acceptor case. Without the tunnel coupling the matrix element for the direct optical transitions between the states $\varphi(\varepsilon)$ and $\xi(\varepsilon')$ is given by

$$M_0(\varepsilon,\varepsilon') = \left\langle \xi(\varepsilon') \left| \hat{M} \right| \varphi(\varepsilon) \right\rangle = u_k \frac{\sqrt{mm'}}{k\hbar^2}\delta(k-k'), \tag{20}$$

where u_k is the appropriate dipole matrix element for the Bloch amplitudes. According to the above mentioned considerations it is only this matrix element that is affected by the tunnel coupling, while the matrix elements for the transitions between higher cylindrical harmonic are preserved. Denoting by M the modified matrix element for transitions between the states $\Psi(E)$ and $\xi(\varepsilon')$ with the further use of the Fano theory [1] one obtains

$$M(E,\varepsilon')^2 = M_0(E,\varepsilon')^2\left[1 - \frac{\pi^2 t^4}{\pi^2 t^4 + (E-\tilde{\varepsilon}_0)^2}\right]. \tag{21}$$

We proceed further with the Fermi's Golden Rule for the transition probability:

$$W(\hbar\omega) = \frac{2\pi}{\hbar}\times$$

$$\times\int_0^\infty\int_0^\infty \left|M(E,\varepsilon')\right|^2 f'(\varepsilon')f(E)\delta(E+\varepsilon'+E_g-\hbar\omega)\,dEd\varepsilon', \tag{22}$$

where E_g is the QW bandgap, $\hbar\omega$ is the energy of the radiated photon, f, f' are the energy distribution functions for the carriers in the hybridized and intact bands, respectively. Substituting (20) and (21) into (22) one should treat correctly the delta-function for the wavenumbers of the zeroth cylindrical harmonic. It can be shown that

$$\delta^2(k-k') = \frac{\sqrt{S}}{\pi^{3/2}}\delta(k-k'),$$

where S is the area of the QW. Then we arrive at

$$W(\hbar\omega) = \frac{u^2 f(E_\omega)}{\pi^{1/2}\hbar^2}\frac{\sqrt{2\tilde{m}S}}{\sqrt{\hbar\omega - E_g}}\left(1 - \frac{\pi^2 t^4}{\pi^2 t^4 + (E_\omega - \tilde{\varepsilon}_0)^2}\right), \tag{23}$$

where

$$f(E_\omega) = f'(\alpha^{-1}E_\omega)f(E_\omega), \qquad E_\omega = \frac{\hbar\omega - E_g}{1+\alpha^{-1}},$$

$$\tilde{m} = \frac{mm'}{m+m'}, \qquad \alpha = \frac{m'}{m}, \tag{24}$$

while for the all cylindrical harmonics altogether the unperturbed optical transition rate yields:

$$W_0(\hbar\omega) = \frac{2\pi u^2 f(E_\omega)}{\hbar}\left(\frac{\tilde{m}}{\hbar^2}S\right). \tag{25}$$

The result (23) obtained for a single impurity can be applied to an ensemble of impurities provided their interaction is weak compared to the tunnel coupling with the QW. In this case the sample area S should be replaced with the inverse sheet concentration of the impurities in the delta-layer n^{-1}. After normalization by the area of the QW from (23), (25) we finally get the spectral density of the luminescence intensity:

$$I(\hbar\omega,\tilde{\varepsilon}_0) = I_0(\hbar\omega)\left(1 - a(\tilde{\varepsilon}_0)\sqrt{n}\frac{\pi^2 t^4}{\pi^2 t^4 + (E_\omega - \tilde{\varepsilon}_0)^2}\right), \tag{26}$$

where

$$a(\tilde{\varepsilon}_0) = \frac{\hbar}{\pi^{3/2}\sqrt{2\tilde{m}\tilde{\varepsilon}_0(1+\alpha^{-1})}},$$

$$I_0(\hbar\omega) = \frac{2\pi u^2 \tilde{m}}{\hbar^3} f(E_\omega).$$

4. Polarization of the spectra

It follows from (26) that the bound state lying within the energy range of the continuum causes a dip in the luminescence spectra emitted from the QW. If then for any reason the bound state is split the luminescence spectra will show the appropriate number of the dips shifted by the splitting energy Δ. If one considers the splitting in the magnetic field applied along z each of the split sublevels is characterized by certain projection of spin and interacts with only one of the 2D carriers spin subbands characterized by the same projection of spin. Thus, for each of the two circular polarizations σ^+, σ^- of the light emitted from the QW one would expect one dip, its spectral position being different for σ^+ and σ^- in accordance with the splitting energy Δ. As an example let us consider the GaAs-based QW and 2D heavy holes interacting via the tunneling configuration interaction with the bound state at an acceptor. This case is shown schematically in Fig. 1. The 2D holes with the projections of total angular momentum $j = +3/2$ and $j = -3/2$ recombine emitting, respectively, right- (σ^+) and left- (σ^-) circularly polarized light. In Sec. 2 it was shown that the heavy holes

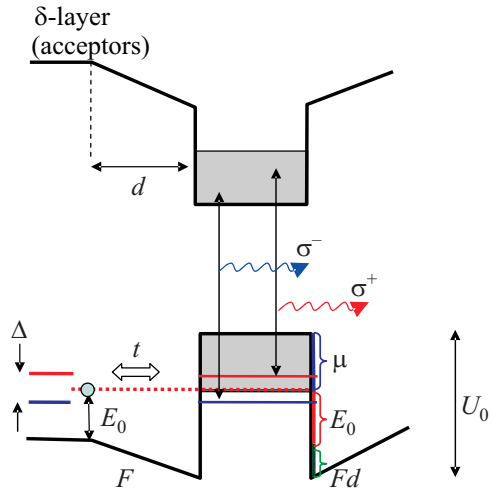

Fig. 1. (Color online) Mechanism of polarization of the luminescence for the acceptor type impurity. The localized hole levels split in magnetic field. Each of them effectively couples with the 2D holes having certain projection of angular momentum. Shifted positions of the resonances with account for temperature distribution of the holes cause the difference in intensities of circular polarizations σ^+, σ^-. The scheme also shows the simple electrostatic model described in the text.

with $j = -3/2\,(j = +3/2)$ interact basically with the bound states $\psi_{-3/2}(\psi_{+3/2})$. An external magnetic field applied along z would cause Zeeman splitting of the bound state energy level ε_0 into $\varepsilon_0^+ = \varepsilon_0 + \Delta/2$ and $\varepsilon_0^- = \varepsilon_0 - \Delta/2$. The splitting $\Delta = \varepsilon_0^+ - \varepsilon_0^-$ may also originate from exchange interaction of the holes with spin-polarized acceptor ions. Let us refer to the case of Mn ions having positive g-factor ($g \approx 3$, see Ref. 11). The hole is coupled to Mn in antiferromagnetic way thus the level ε_0^+ corresponds to $j = -3/2$ and ε_0^- to $j = +3/2$. As follows from (17), (24) the difference in the positions of the resonances (dips) E_ω^+ and E_ω^- corresponding to the bound state sublevels ε_0^+ and ε_0^- is given by

$$\tilde{\Delta} = E_\omega^+ - E_\omega^- = \Delta + t^2 \ln\left(1 + \frac{\tilde{\Delta}}{E_\omega^-}\right). \qquad (27)$$

Unless the positions of the resonances are too close to the band edge the last term in (26) can be neglected and $\tilde{\Delta} = \Delta = \varepsilon_0^+ - \varepsilon_0^-$. With account for the energy distribution functions for the holes and electrons the shifted positions of the resonances lead to the difference in the luminescence intensity for the opposite circular polarizations. In the discussed example of the antiferromagnetic alignment of the hole the luminescence spectra $I^+(\hbar\omega, \tilde{\varepsilon}_0^+)$, $I^-(\hbar\omega, \tilde{\varepsilon}_0^-)$ having the resonance positions at ε_0^+ and ε_0^- correspond to the circular polarizations σ^- and σ^+, respectively. As can be seen from (26) the difference in the resonance positions $\Delta = \tilde{\varepsilon}_0^+ - \tilde{\varepsilon}_0^-$ leads to the integral polarization of the spectra if the distribution function $f(E)$ significantly varies in the vicinity of ε_0. This is illustrated in Fig. 2. The functions I^- and I^+ are shown by blue and red solid lines, respectively. The integral polarization is naturally defined as

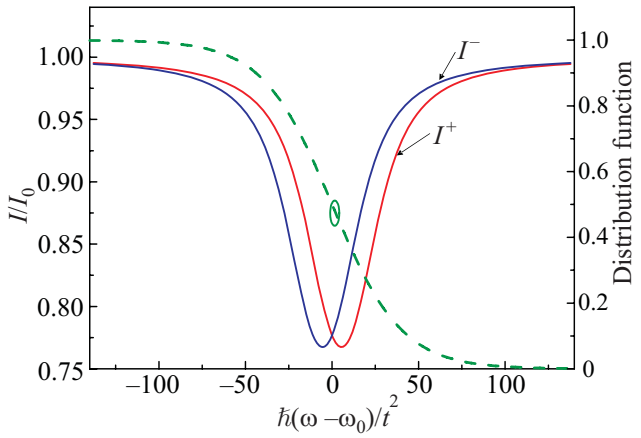

Fig. 2. (Color online) Modification of the luminescence spectrum by tunneling configuration interaction. The integral polarization occurs when the carriers distribution function (dashed line) strongly varies in the vicinity of the configuration resonances. ω_0 is the position of the resonance without bound level splitting.

$$P = \frac{P(\sigma^+) - P(\sigma^-)}{P(\sigma^+) + P(\sigma^-)} \approx \frac{\int\limits_{E_g}^{\infty} I^-(\hbar\omega)\, d(\hbar\omega) - \int\limits_{E_g}^{\infty} I^+(\hbar\omega)\, d(\hbar\omega)}{2\int\limits_{E_g}^{\infty} I_0(\hbar\omega)\, d(\hbar\omega)}.$$

With use of (26) this yields:

$$P = -\sqrt{n}\,\frac{\int\limits_0^{\infty} \pi t^2(E)\left[\dfrac{a(\tilde{\varepsilon}_0^+)\pi t^2(E)}{\pi^2 t^4(E) + (E-\tilde{\varepsilon}_0^+)^2} - \dfrac{a(\tilde{\varepsilon}_0^-)\pi t^2(E)}{\pi^2 t^4(E) + (E-\tilde{\varepsilon}_0^-)^2}\right] f(E)dE}{2\int\limits_0^{\infty} f(E)dE}. \tag{28}$$

The slow varying functions $f(E)$ and $\tilde{\varepsilon}_0(E)$ in the integral may be assumed as constants taken at $\tilde{\varepsilon}_0^-$, $\tilde{\varepsilon}_0^+$, the tunneling parameter will be treated as a constant in the whole range of interest $t^2(E) \equiv t^2$.

Then treating the expression in brackets as delta-functions we obtain

$$P = -\frac{\sqrt{\pi}\hbar t^2\sqrt{n}}{2^{3/2}\sqrt{m}}\,\frac{f(\varepsilon_0^+)(\varepsilon_0^+)^{-1/2} - f(\varepsilon_0^-)(\varepsilon_0^-)^{-1/2}}{\int\limits_0^{\infty} f(E)dE}. \tag{29}$$

Note that for the considered example the polarization degree appears to be negative. The positive sign would have appeared if the ferromagnetic coupling between the acceptor ion and the hole had been assumed.

5. The electrostatic effect

Because of the tunneling involved in the polarization of the luminescence one might reasonably expect very strong dependence of the polarization degree on the distance d between the δ-layer and the QW (i.e., the thickness of the spacer). However, the purely exponential dependence of the polarization on the barrier thickness appears to be weakened due to the electrostatic effect shown in Fig. 1 and explained below. Let us for simplicity consider the electrons distribution function being nearly constant within the configuration resonances. The holes are considered to have Fermi distribution function characterized by the chemical potential μ and the temperature T. In the absence of external optical pumping the holes in the QW are in thermodynamic equilibrium with the acceptors in the δ-layer, therefore they have the same chemical potential. Under low-pumping conditions the already large concentration of the holes in the QW is not strongly violated, so it is reasonably to assume that the quasi-Fermi levels of the holes at the acceptors and in the QW coincide, it means that $\varepsilon_0 = \mu$. Strictly speaking, this is valid for a single bound level, if the level is split so that $\varepsilon_0^+ - \varepsilon_0^- = \Delta$, one should probably assume $\varepsilon_0^- = \mu$. From (29) we get the following simplified expression:

$$P = -\frac{\sqrt{\pi}\hbar t^2\sqrt{n}}{2^{5/2}\sqrt{m'_{hh}}\,\mu^{3/2}}\tanh\frac{\Delta}{2kT}. \tag{30}$$

As we will show below both t and μ contribute to the dependence of the integral polarization P on the spacer thickness d and the QW depth U_0. The holes in the QW provide an electrical charge density estimated as $\sigma = eN\mu$, where e is the elementary charge, N is the 2D density of states. The positively charged plane of the QW and negatively charged δ-layer of partly ionized acceptors separated by a distance d produce an electric field

$$F = \frac{4\pi eN\mu}{\varepsilon}, \tag{31}$$

ε being dielectric constant of the material. Due to the electric field F the valence band edge at position of the impurities delta-layer appears to be shifted from the valence band edge just outside of the QW by $F \cdot d$. Because the quasi-Fermi level of the acceptors exceeds the local position of the valence band edge by the binding energy E_0, the equality of the quasi-Fermi levels leads to a simple equation (see Fig. 1):

$$U_0 = \mu + E_0 + eFd, \tag{32}$$

where U_0 is the QW depth and μ is the chemical potential of the holes in the QW. With (31) one gets

$$\mu = \frac{U_0 - E_0}{1 + 4\pi Ned/\varepsilon} \approx \frac{(U_0 - E_0)\varepsilon}{4\pi Ned}. \tag{33}$$

In order to estimate the dependence of the tunneling parameter t on the QW and spacer parameters we consider the WKB tunneling through trapezoid barrier as seen in Fig. 1. With taking into account (12) and (33) this leads to the following expression (we assume $\mu \ll U_0$):

$$t^2 \sim \exp(-\kappa d), \tag{34}$$

where

$$\kappa = \frac{4\sqrt{2m_{lh}}}{3\hbar(U_0 - E_0)}(U_0^{3/2} - E_0^{3/2}). \qquad (35)$$

From (20), (33)–(35) follows the dependence of integral polarization on the spacer thickness:

$$P \sim d^{3/2} \exp(-\kappa d). \qquad (36)$$

Note that electrostatic effect results in the dependence of μ on d which leads to the dependence of P on d being not purely exponential but weakened by the pre-exponential factor $d^{3/2}$. While the correction is pre-exponential, it appears to be quite impotant up to $\kappa d \approx 2$–3 which is typical for the experimental situation.

6. Discussion

In the proposed theory the polarization of light emitted from the QW originates from the splitting of the impurity bound state and therefore may exceed the polarization degree expected from an intrinsic g-factor of the 2D carriers located in the QW. The sign of the polarization deserves special discussion. As was shown above, the tunnel coupling causes a dip in the luminescence spectra. This means that in the considered scheme the polarization of the luminescence from the QW is expected to be of the opposite sign than that due to the optical transitions between the bound state and the free carriers inside the barrier. In particular, the configuration interaction between the 2D heavy holes and Mn δ-layer considered in Sec. 4 leads to the negative sign of the polarization (a mistake made in Ref. 10 has mislead to the positive sign). Such result contradicts the known experimental data [12,13], where the polarization is shown to be positive. This might suggest that regarding these particular experiments the polarization is not due to the holes configuration interaction but rather due to polarization of the electrons as suggested in Ref. 13. The other possibility might be that the relevant bound state of the hole at Mn is more complex and does not resemble the simple antiferromagnetic exchange coupling with Mn ion.

Let us estimate the expected magnitude of the circular polarization degree due to the tunnel configuration interaction. We assume the deep impurity level $E_0 = 100$ meV, the barrier thickness $d = 5$ nm, the QW width $a = 10$ nm. Taking the effective mass as that of the electrons in GaAs $m = 0.06\, m_0$ for the simple band case described by (8) one gets for the tunneling parameter $(t^e)^2 \approx 2$ meV. The estimation for the holes tunneling parameter appears to be far less, taking $m_{hh} = 0.5\, m_0$, $m'_{hh} = 0.15\, m_0$ from (12) one gets $(t^h)^2 \sim 0.01$ meV. The polarization degree is to be estimated using (29). We take $\Delta = 1$ meV, $T_e = T_h = 20$ K, the sheet concentration of the impurities $n = 10^{13}$ cm^{-2}. Then for the case of the donor impurity $t = t^e$, $\varepsilon_0 = 4$ meV, $\mu_h = -1$ meV, $\mu_e = \varepsilon_0^-$, one gets $|P| \approx 40\%$, for the acceptor impurity $t = t^h$, $\mu_e = -1$ meV, $\varepsilon_0 = 2$ meV, $\mu_h = \varepsilon_0^-$ gives $|P| \approx 0.5\%$. An illustration of the luminescence spectra for the two circular polarizations is presented Fig. 3. For this we used an intermediate value for the tunneling parameter $t^2 = 0.3$ meV ($|P| \approx 0.15\%$) and accounted for inhomogeneous broadening of the spectra by normal distribution of the bandgap E_g with the dispersion $\sigma = 3$ meV (corresponds to the fluctuation of the QW width by half a monolayer).

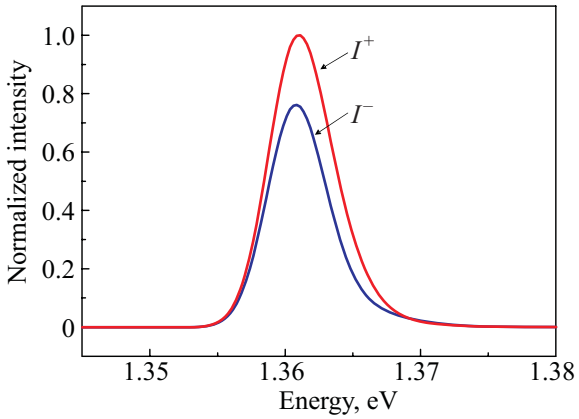

Fig. 3. (Color online) An example of calculated luminescence spectra for the two circular polarizations. The case of antiferromagnetic coupling implies I^- corresponds to σ^+ polarization while I^+ to σ^- polarization. The parameters used in calculations are given in the text.

7. Summary

The presented theory describes the tunnel coupling between a continuum of states in the QW and an impurity bound state located outside of the QW. We utilized the well known Fano approach for calculation of the matrix elements for the direct interband optical transitions in the QW. For such transitions the tunnel coupling of the 2D QW states with the impurity states leads to the drop of the luminescence spectral density at the frequency corresponding to the configuration resonance. This modification of the spectra leads to an integral circular polarization of the light emitted from the QW provided the bound hole state is split in the projection of the hole angular momentum. The key advantage of the approach used in the present study is that the unknown eigenfunctions of the system are expressed through those of the uncoupled states. Given the expansion (13) any effects on the localized state can be translated into effects for the whole coupled system. For this reason it is capable of describing other effects expected in such systems like anisotropy of the holes g-factor in the QW induced by the paramagnetic impurity or the indirect exchange interaction between the bound states provided by the 2D free carriers in the QW.

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