

Tunneling magnetic effect in heterostructures with paramagnetic impurities

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An effect of paramagnetic impurity located in a vicinity of a quantum well (QW) on spin polarization of the carriers in the QW is analyzed theoretically. Within the approach of Bardeen's tunneling Hamiltonian the problem is formulated in terms of the Anderson-Fano model of configuration interaction between a localized hole state at Mn and continuum of heavy hole states in the InGaAs-based QW. The hybridization between the localized state and the QW leads to resonant enhancement of interband radiative recombination. The splitting of the configuration resonances induced by splitting of the localized state in magnetic field results in circular polarization of light emitted from the QW. The developed theory is capable of explaining known experimental results and allows for calculation of the photoluminescence spectra and dependence of integral polarization on temperature and other parameters.

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I. INTRODUCTION

Various phenomena based on the interference of a bound quantum-mechanical state and continuum states have been intensively studied since the famous paper by Fano¹ rated among the most relevant works of 20th century.² He suggested a theoretical approach often regarded as the Fano-Anderson model or Fano configuration interaction which succeeded in explaining asymmetric resonances observed in atomic spectroscopy experiments. It further appeared that numerous examples of Fano resonances existed in atomic and nuclear physics, condensed matter physics, and optics.² The coexistence 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. Such structures are believed to combine high mobility of the carriers in the QW and magnetic properties provided by the magnetic layer. In particular, an exchange interaction with ferromagnetic layer leads to spin polarization of holes.⁶ For GaAs-based structures with an Mn δ layer the holes probably play an important role in promoting a ferromagnetic state of the Mn layer.^{7,8} The system considered in the present work consists of a GaAs-based heterostructure with $\text{In}_x\text{Ga}_{1-x}\text{As}$ QW ($x = 0.1 - 0.2$) and a δ layer of paramagnetic acceptors (Mn) located at a distance of several nanometers from the QW. 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.^{9,10} It was found that the PL intensities at wavelength corresponding to interband direct transitions in the QW differ for opposite circular polarizations. If Mn is replaced by a nonmagnetic acceptor (carbon) the polarization decreases dramatically. Thus the polarization is not due to the intrinsic g factor of the two-dimensional (2D) carriers in the QW which in this way is proved to be small. On the contrary, the holes localized at Mn do have $g \approx 3$ (see Ref. 11) and possibly can penetrate into the QW by means of the quantum-mechanical tunneling which is expected to be of a resonant type if the energy of the localized state

coincides with that of the free 2D hole in the QW. The purpose of our work is to establish a proper theory capable of describing the polarization of the PL emitted from the QW induced by paramagnetic impurity by means of weak tunnel coupling. Figure 1 shows schematically a band diagram of the considered system. To study tunnel hybridization between the localized hole state at Mn and the 2D continuum states in the QW we utilize the Fano configuration interaction approach¹ and show how this hybridization reveals itself in the photoluminescence at the QW wavelength. In our theory the circular polarization in the external magnetic field appears in the following manner. An external magnetic field splits the localized level of the hole sitting at Mn. The splitting Δ could be either due to a conventional Zeeman effect or caused by the p - d exchange interaction with Mn electrons. For each of the split levels the tunnel coupling occurs with only one (of the two having opposite spin projections) 2D heavy hole subbands in the QW. As a result the distribution of holes appears to be different in the two subbands resulting in different intensities of σ^+ and σ^- polarized light emitted from the QW.

We have to mention here that while the considered mechanism based on the holes tunneling is quite naturally expected in the p -type system, there are other mechanisms that might contribute to the experimentally observed polarization. One of those is nonresonant tunneling of electrons from QW to Mn followed by recombination with the holes localized at Mn. Up to now it still remains unclear which of the mechanisms has larger contribution to the polarization in experiments on photoluminescence.^{9,10} In our paper we focus only on the mechanism related to the holes' resonant tunneling and therefore for making things more clear we assume that the 2D electrons are localized in the QW and do not penetrate to the impurity site (e.g., due to the high offset of the conductance band).

The paper is organized as follows. In Sec. II we consider one bound hole state at the acceptor and the 2D states in the QW being decoupled from each other. In Sec. III we study hybridization of the bound state with the 2D continuum states by means of tunnel configuration interaction. Finally, the effect

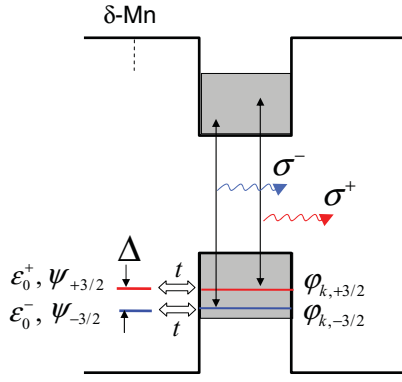


FIG. 1. (Color online) Mechanism of polarization of the luminescence. The localized hole levels split in magnetic field. Each of them effectively couples with the 2D holes having certain projection of angular momentum. Shifted positions of the resonances with account for temperature distribution of the holes cause the difference in intensities of circular polarizations σ^+ , σ^- .

of the hybridization on the PL polarization in the magnetic field is discussed in Secs. IV and V.

II. HOLE STATES AT ACCEPTOR AND IN QUANTUM WELL

In this section we consider the bound state of a hole at an acceptor and the 2D QW states independently as if they were separated by an infinitely wide potential barrier. Nevertheless, it is worth remembering that the whole system under study (impurity + QW) has cylindrical symmetry with the cylindrical axis z 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 wave number k and the cylindrical harmonic number l . The corresponding wave function normalized by a circle of an area S is given by

$$\varphi_{kl}(\rho, \theta, z) = \eta(z) \frac{\pi^{1/4} \sqrt{k}}{\sqrt{2} S^{1/4}} J_l(k\rho) e^{il\theta}, \quad (1)$$

where $J_l(k\rho)$ is the Bessel function of order l , ρ and θ are the polar coordinates in the QW plane, $\eta(z)$ is the envelope function of size quantization in the z direction. The wave function is normalized to unity. Firstly, let us treat this continuum as a set of discrete states, each characterized by its energy ε_k and its wave function φ_{kl} . Considering the 2D carriers as free implies that the magnetic field applied to the QW is nonquantizing. The validity of this assumption is discussed in Sec. V. Below we consider $\text{In}_x\text{Ga}_{1-x}\text{As}$ QW having only one level of size quantization for the heavy holes; we 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 the z axis which is perpendicular to the QW plane:

$$(e_{3/2}, e_{1/2}, e_{-1/2}, e_{-3/2}). \quad (2)$$

The wave functions describing the heavy holes in this basis have the form,

$$\varphi_{kl, -\frac{3}{2}} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \varphi_{kl}(\rho) \end{pmatrix}, \quad \varphi_{kl, +\frac{3}{2}} = \begin{pmatrix} \varphi_{kl}(\rho) \\ 0 \\ 0 \\ 0 \end{pmatrix}. \quad (3)$$

The kinetic energy of the 2D QW state is related to k as

$$\varepsilon = \frac{\hbar^2 k^2}{2m'_{hh}}, \quad (4)$$

where m'_{hh} is the in-plane heavy hole mass in the QW.

In order to determine wave function ψ of a hole localized at an acceptor one should consider the kinetic part of the Luttinger Hamiltonian and attractive potential of the acceptor $U(r)$. The spherically symmetrical potential preserves the symmetry Γ_8 , thus the ground state is fourfold degenerate and can be classified by angular momentum projection. The eigenfunctions of Luttinger Hamiltonian with spherically symmetric attractive potential can be explicitly found in the model of zero radius potential.¹² In the basis of the Bloch amplitudes they are expressed as follows:

$$\begin{aligned} \psi_{+\frac{3}{2}} &= \begin{pmatrix} R_0 Y_{00} + \frac{1}{\sqrt{5}} R_2 Y_{20} \\ -\frac{2}{\sqrt{10}} R_2 Y_{21} \\ \frac{2}{\sqrt{10}} R_2 Y_{22} \\ 0 \end{pmatrix}, \\ \psi_{+\frac{1}{2}} &= \begin{pmatrix} \frac{2}{\sqrt{10}} R_2 Y_{2,-1} \\ R_0 Y_{00} - \frac{1}{\sqrt{5}} R_2 Y_{20} \\ 0 \\ \frac{2}{\sqrt{10}} R_2 Y_{22} \end{pmatrix}, \\ \psi_{-\frac{1}{2}} &= \begin{pmatrix} \frac{2}{\sqrt{10}} R_2 Y_{2,-2} \\ 0 \\ R_0 Y_{00} - \frac{1}{\sqrt{5}} R_2 Y_{20} \\ \frac{2}{\sqrt{10}} R_2 Y_{21} \end{pmatrix}, \\ \psi_{-\frac{3}{2}} &= \begin{pmatrix} 0 \\ \frac{1}{\sqrt{5}} R_2 Y_{2,-2} \\ -\frac{2}{\sqrt{10}} R_2 Y_{2,-1} \\ R_0 Y_{00} + \frac{1}{\sqrt{5}} R_2 Y_{20} \end{pmatrix}. \end{aligned} \quad (5)$$

Here

$$\begin{aligned} R_0 &= C_0 \left(\frac{\beta}{r} e^{-qr\sqrt{\beta}} + \frac{e^{-qr}}{r} \right), \\ R_2 &= C_0 \left(\frac{\beta}{r} e^{-qr\sqrt{\beta}} \left(1 + \frac{3}{qr\sqrt{\beta}} + \frac{3}{q^2 r^2 \beta} \right) - \frac{e^{-qr}}{r} \left(1 + \frac{3}{qr} + \frac{3}{q^2 r^2} \right) \right), \\ C_0 &= \sqrt{\frac{q}{\beta^{3/2} + 1}}, \quad q = \sqrt{\frac{2m_{hh} E_0}{\hbar^2}}, \quad \beta = \frac{m_{lh}}{m_{hh}}. \end{aligned} \quad (6)$$

E_0 is the binding energy of the hole at the acceptor; Y_{lm} are the spherical harmonics. m_{lh} , m_{hh} , respectively, are the bulk light hole mass and the heavy hole mass in GaAs. Note that the radial part of all nonzero components of the wave functions (5) have two characteristic decay lengths, the largest of the

two being always determined by the light hole mass $m_{lh} \approx 0.08 m_0$, where (m_0 is the free electron mass).

III. TUNNELING BETWEEN ACCEPTOR AND QUANTUM WELL

With ionization energy of Mn being of the order of $E_0 \sim 100$ meV and the width of the potential barrier separating the Mn δ layer from the QW of the order of $d \sim 3$ nm one can estimate the tunneling transparency of the barrier for the light hole as $\exp(-2\frac{\sqrt{2m_{lh}E_0}}{\hbar}d) \approx 0.05$. With that, the barrier appears to be weakly transparent and one can get use of the so-called tunneling Hamiltonian (or transfer Hamiltonian) formalism originally proposed by Bardeen.¹³ In this approach the total Hamiltonian of the system is expressed as follows:

$$H = \varepsilon_0 a^+ a + \sum_{k,l} \varepsilon_k c_{kl}^+ c_{kl} + \sum_{k,l} (T_{kl} c_{kl}^+ a + T_{kl}^* a^+ c_{kl}), \quad (7)$$

where a^+, a are the creation and annihilation operators for the localized state characterized by its energy ε_0 , and c_{kl}^+, c_{kl} are the creation and annihilation operators for the 2D QW state characterized by its wave number k and the cylindrical harmonic number l . The energy here and below is measured from the 2D hole size quantization level, therefore ε_k is given by (4). The tunneling parameter T_{kl} describes the tunnel coupling between the localized state and the QW state. Our analysis will be focused on the case of the hole's kinetic energy being substantially less than the binding energy E_0 (i.e., $k \ll q$). From Eqs. (1), (3), and (5) it follows that for this case the overlap integrals involving φ_{kl} with $l \neq 0$ are suppressed by a small parameter k/q . It means that for the studied case only the zeroth cylindrical harmonic should be taken into account. For $k \ll q$ it is also reasonable to assume that $T_k \equiv T_{k0}$ does not depend on k . Still, its rapidly decreasing behavior for $k \gg q$ has to be kept in mind when it provides convergence for integration over k . Interaction with only the zeroth harmonic means that the continuum spectrum modified by tunneling is nondegenerate. This fact is not essential for the qualitative results obtained below, but simplifies the calculations. Finally, we conclude that the tunneling configuration interaction to be accounted for is only between $\varphi_{k0,-\frac{3}{2}}$ and $\psi_{-\frac{3}{2}}$, and between $\varphi_{k0,+\frac{3}{2}}$ and $\psi_{+\frac{3}{2}}$. Both are governed by the same tunneling parameter T_k which in the framework of the Bardeen's approach can be estimated as

$$T_k \sim \frac{\hbar^2}{2m_0} \frac{q\sqrt{k}}{S^{1/4}} \exp(-qd\sqrt{\beta}). \quad (8)$$

The tunneling parameter T_k exponentially depends on the barrier thickness with the light hole mass entering the exponent index.

The transfer Hamiltonian (7) with known tunneling parameter (8) allows one to apply the Fano-Anderson model¹³ and construct eigenfunctions Ψ of the whole system from those of the localized state ψ and the QW states φ_k :

$$\Psi(E) = v_0(E)\psi + \sum_k v_k(E)\varphi_k, \quad (9)$$

where E denotes the energy of the state Ψ . Here φ_k are the QW wave functions of the zeroth cylindrical harmonic $\varphi_k = \varphi_{k0}$.

Plugging (9) into the stationary Schrodinger equation,

$$H\Psi = E\Psi,$$

with H being the effective Hamiltonian (7) one gets the following system of linear equations:

$$v_0\varepsilon_0 + \sum_k v_k T_k^* = E v_0, \quad v_k \varepsilon_k + T_k v_0 = E v_k. \quad (10)$$

Solving the eigenvalue problem for (10) one can get the spectrum and the coefficients v_0, v_k (i.e., the eigenfunctions of the system). Transition from the discrete set of states $v_k(E)$ to the continuous function $v(\varepsilon, E)$ is straightforward (as the continuum states are nondegenerate we can use the energy ε instead of k as the quantum number). Instead of (9) and (10) we write

$$\Psi(E) = v_0(E)\psi + \int_0^\infty v(E, \varepsilon)\varphi(\varepsilon)d\varepsilon, \quad (11)$$

$$v_0(E)\varepsilon_0 + \int_0^\infty t(\varepsilon)v(E, \varepsilon)d\varepsilon = E v_0(E), \quad (12)$$

$$v(E, \varepsilon)\varepsilon + t(\varepsilon)v_0(E) = E v(E, \varepsilon).$$

The normalizations for ψ and $\varphi(\varepsilon)$ are

$$\langle \psi(\varepsilon_0) | \psi(\varepsilon_0) \rangle = 1, \quad \langle \varphi(\varepsilon) | \varphi(\varepsilon') \rangle = \delta(\varepsilon - \varepsilon'). \quad (13)$$

With the chosen normalization, the discrete tunneling parameter T_k and the one entering (12) are related as follows:

$$T_k^2 N_0(\varepsilon) = t^2(\varepsilon), \quad (14)$$

where

$$N_0(\varepsilon) = \sqrt{\frac{m_{hh} S}{2\pi^3 \varepsilon \hbar^2}} \quad (15)$$

is the density of states with the zeroth cylindrical harmonic. The discrete system (10) is an eigenvalue problem, but the continuous problem (12) is not. In the present work we consider the case of the localized energy level lying within the range of the continuum states: $\varepsilon_0 \gg t^2$. For this case the solution of (12) can be obtained in the form,¹

$$v_0^2(E) = \frac{t^2(E)}{\pi^2 t^4(E) + (E - \tilde{\varepsilon}_0)^2}, \quad (16)$$

$$v(E, \varepsilon) = v_0(E) \left(P \frac{t(\varepsilon)}{E - \varepsilon} + Z(E) t(E) \delta(E - \varepsilon) \right),$$

where

$$Z(E) = \frac{E - \varepsilon_0 - F(E)}{t^2(E)}, \quad F(E) = P \int_0^\infty \frac{t^2(\varepsilon)}{E - \varepsilon} d\varepsilon. \quad (17)$$

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 :

$$\tilde{\varepsilon}_0(E) = \varepsilon_0 + F(E). \quad (18)$$

Because of $k \ll q$ it is reasonable to treat $t = \text{const}$ everywhere, except for (17) where decrease of t at $E \rightarrow \infty$ is necessary for the integral convergence. In order to analyze the influence of the configuration interaction on the luminescence spectra we have to calculate matrix element of the operator

\hat{M} describing interband radiative transitions between the hybridized hole wave function $\Psi(E)$ and the wave function of an electron in the QW of the conductance band $\xi_{k_e l_e}$; here k_e is the electron wave number, and l_e is the cylindrical harmonic number analogously to (1). As was already discussed in Sec. I we assume that (a) there are no radiative transitions between the localized hole wave function ψ and the 2D electron wave function $\xi_{k_e l_e}$, (b) the interband radiative transitions between the free 2D states in the QW are direct. The appropriate matrix elements are therefore given by

$$\langle \xi_{k_e l_e} | \hat{M} | \psi \rangle = 0, \quad (19)$$

$$M_0 = \langle \xi_{k_e l_e} | \hat{M} | \varphi_{kl} \rangle = u_k \delta(k - k_e) \delta_{l, l_e}, \quad (20)$$

where u_k is the appropriate dipole matrix element. With use of Eqs. (11), (16), (19), and (20) we arrive at the matrix element for the transitions between the states $\Psi(E)$ and $\xi_{k_e 0}$ (according to previous notes this matrix element differs from M_0 only for the zeroth cylindrical harmonic):

$$M = \langle \xi_{k_e 0} | \hat{M} | \Psi(E) \rangle = v(E, \alpha \varepsilon_e) u(\alpha \varepsilon_e), \quad (21)$$

$\alpha = m_e / m'_{hh}$, where m_e is the effective in-plane electron mass, $\varepsilon_e = \hbar^2 k_e^2 / 2m_e$. The particular form of M (21) prevents from calculation of the ratio M^2 / M_0^2 as done in the classical Fano resonance calculations.¹ The latter assume unperturbed matrix element M_0 to be constant. This is obviously not the case for the direct optical transitions demanding momentum conservation (20). In our case the ratio M^2 / M_0^2 doesn't readily give a physically meaningful result due to the delta function in Eq. (16); one rather has to proceed to calculation of an observable. With the Fermi's Golden Rule for the transition probability we write

$$W(\hbar\omega) = \frac{2\pi}{\hbar} \int_0^\infty \int_0^\infty |M(E', \varepsilon_e)|^2 f_e(\varepsilon_e) f_h(E') \times \delta(E' + \varepsilon_e + E_g - \hbar\omega) dE' d\varepsilon_e, \quad (22)$$

where E_g is the bandgap, $\hbar\omega$ is the energy of the radiated photon, and f_e, f_h are the energy distribution functions for the electrons and holes, respectively. To deal properly with the delta function entering M^2 in Eq. (21) and emerging in Eq. (22) we pass on to averaging $W(\hbar\omega)$ over a small spectral interval of the width Ω centered at ω_0 :

$$\tilde{W}(\hbar\omega_0) = \frac{1}{\Omega} \int_{\omega_0 - \Omega/2}^{\omega_0 + \Omega/2} W(\hbar\omega) d\omega.$$

Using Eqs. (21) and (16) we obtain

$$\begin{aligned} \tilde{W}(\hbar\omega_0) &= \frac{2\pi}{\hbar} \frac{1}{\hbar\Omega} \int_{\frac{\hbar\omega_0 - E_g - \hbar\Omega/2}{1+\alpha^{-1}}}^{\frac{\hbar\omega_0 - E_g + \hbar\Omega/2}{1+\alpha^{-1}}} \\ &\times \left[N(E') - \frac{1}{t^2(E')(\pi^2 + Z^2(E'))} \right] \\ &\times u^2(\alpha^{-1} E') f(E') dE', \end{aligned} \quad (23)$$

where

$$f(E') = f_e(\alpha^{-1} E') f_h(E'). \quad (24)$$

The first term in brackets describes the transition rate for radiative recombination in the QW with no account for the tunneling, therefore $N(E')$ here is the total density of states (including not only the zeroth but all cylindrical harmonics):

$$N(E') = \frac{m'_{hh} S}{2\pi \hbar^2}. \quad (25)$$

Integration assuming the functions $\tilde{\varepsilon}_0, t, u, f$ being constant within the range of integration [$t(E) \equiv t$, $u(E) \equiv u$ are assumed constant everywhere] yields

$$\begin{aligned} \tilde{W}(\hbar\omega_0) &= \frac{2\pi}{\hbar} u^2 f(E) \left[\frac{m'_{hh} S}{2\pi \hbar^2} - \frac{1}{\hbar\Omega\pi} \left[\arctan \frac{\Delta E + w}{\pi t^2} \right. \right. \\ &\quad \left. \left. - \arctan \frac{\Delta E - w}{\pi t^2} \right] \right], \end{aligned} \quad (26)$$

where

$$E = \frac{\hbar\omega_0 - E_g}{1 + \alpha^{-1}}, \quad \Delta E = E - \tilde{\varepsilon}_0(E), \quad w = \frac{\hbar\Omega}{2(1 + \alpha^{-1})}. \quad (27)$$

As we consider the weak tunneling, t^2 is the smallest energy scale. In the vicinity of resonance,

$$\Delta E \in (-w + t^2, w - t^2), \quad (28)$$

expansion of Eq. (26) to the first order in t^2 gives

$$\begin{aligned} \tilde{W}(\hbar\omega_0) &= \frac{2\pi}{\hbar} u^2 f(E) \\ &\times \left[\frac{m'_{hh} S}{2\pi \hbar^2} - \frac{1}{\hbar\Omega} + \frac{1}{1 + \alpha^{-1}} \frac{t^2}{w^2 - (\Delta E)^2} \right]. \end{aligned} \quad (29)$$

Note that Eq. (29) has term $-1/\hbar\Omega$ which does not depend on the tunneling. Its appearance is due to a peculiarity of the mathematics of the Fano model reflected in Eq. (16). When a noninteracting state with energy ε_0 is appended to the system so that ε_0 lies within its spectrum, one of the energy levels of the whole system becomes doubly degenerate. This fact is not properly accounted for in Eq. (16) and one state is lost. It should be added back manually to the spectral density by canceling the second term in Eq. (29). Treating the same issue in a different way, one should examine $\Delta \tilde{W} = \tilde{W} - \tilde{W}_0$ instead of \tilde{W} itself, \tilde{W}_0 being the unperturbed transition rate [Eq. (26) evaluated for $t = 0$]. In a similar way studying the ratio of matrix elements in the original Fano work¹ circumvents the disappearance of one level.

The results obtained for a single impurity can also be applied to an ensemble of impurities provided their interaction between each other is weak compared to the tunnel coupling with the QW. If the concentration of the impurities is low enough to produce only weak perturbation of the luminescence spectra, we can simply multiply the tunneling term by the number of impurities. After normalization by the area of the QW we finally get the spectral density of the luminescence intensity:

$$I(\hbar\omega_0) = \frac{2\pi}{\hbar} u^2 f(E) \left[\frac{m'_{hh}}{2\pi \hbar^2} + \frac{n}{\pi \hbar\Omega} \left[\arctan \frac{\Delta E - w}{\pi t^2} - \arctan \frac{\Delta E + w}{\pi t^2} - \pi \frac{\text{sgn}(\Delta E - w) - \text{sgn}(\Delta E + w)}{2} \right] \right], \quad (30)$$

where n is the surface concentration of the impurities. The last term in brackets corrects the lost level issue to provide exact canceling of the perturbation of the spectra at $t = 0$. For high concentration of the impurities the formula (30) may give a meaningless result (the intensity may become negative at some points). Indeed for high concentration the real physical picture becomes slightly different—interaction between the impurities splits their energy levels forming a small range of discrete levels, accordingly, the configuration resonances become slightly shifted. Taking this effect into account eliminates the puzzling behavior of (30) at high concentration but does not affect the answer for the polarization degree given in the next section.

The obtained analytical result (30) was verified by numerical simulation performed for the discrete system (10). The system was solved for 500 discrete levels with interlevel separation 10^{-5} eV, and the discrete tunneling parameter was taken as $T_k = 3.3 \times 10^{-5}$ eV; this corresponds to the continuous tunneling parameter being $t^2 = 10^{-4}$ eV. The other relevant parameters were as follows: $w = 5 \times 10^{-4}$ eV, $n = 10^{10}$ cm $^{-2}$, $m_e = 0.03 m_0$, $m_{hh} = 0.5 m_0$, $m'_{hh} = 0.15 m_0$. In both calculations all the states were assumed fully occupied [i.e., the energy distribution function was kept $f(E) = 1$]. Analogously to (20) the matrix element for the discrete system was taken: $M_k(\varepsilon, \varepsilon_e) = u_k \delta_{k,k_e} \delta_{l,l_e}$. The calculation result presented in Fig. 2 demonstrates perfect agreement with the analytical expression (30) and confirms the validity of the latter. Both approaches demonstrate that the tunnel configuration interaction gives rise to the luminescence intensity within a certain spectral range (28) near ω_0 . This increase is compensated by the decrease outside of this range as can be seen in Fig. 2. The width of the resonance is determined by Ω which has the meaning of spectral resolution of the measurement setup. However, for comparison with experimental spectra the inhomogeneous broadening should be accounted for as it usually exceeds the instrumental spectral resolution. An expression for the integral intensity

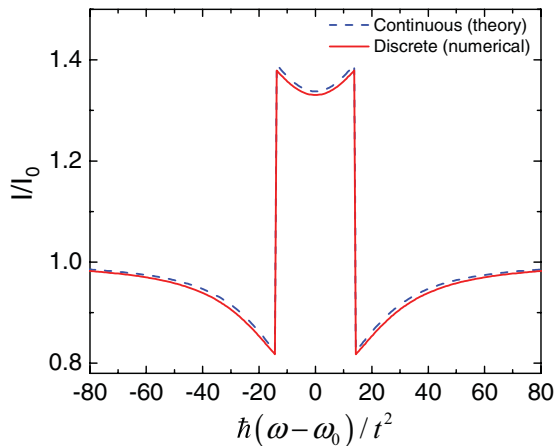


FIG. 2. (Color online) Modification of the luminescence spectrum by tunneling configuration interaction: numerical calculation for the discrete levels (solid line) and analytical formula (30) (dashed line).

over the whole spectra reads

$$I = \frac{2\pi}{\hbar} \int_0^\infty u^2 f(E) \left[\frac{m'_{hh}}{2\pi\hbar^2} - \frac{nt^2(E)}{\pi^2 t^4(E) + (E - \tilde{\varepsilon}_0)^2} + n\delta(E - \tilde{\varepsilon}_0) \right] dE. \quad (31)$$

This formula follows from (22) in the same way as (26) and (29) were obtained. The delta function here is added manually to treat the lost level issue—it provides canceling of the second term in the limit $t \rightarrow 0$ and thus gives the correct expression in the absence of the tunneling:

$$I_0 = \frac{2\pi}{\hbar} \int_0^\infty u^2 f(E) \frac{m'_{hh}}{2\pi\hbar^2} dE. \quad (32)$$

Note that the spectral width of the resonance Ω does not enter the expression for the integral intensity (31).

IV. POLARIZATION OF THE SPECTRA

The redistribution of the PL intensity near the energy corresponding to the bound level does not change the integral intensity but it causes the polarization in the magnetic field as illustrated by 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^-) hand circularly polarized light. In Sec. III it was shown that the heavy holes with $j = -3/2$ interact basically with the bound state $\psi_{-3/2}$. Let us denote the energy of this state as ε_0^- . The 2D holes with $j = +3/2$ interact in turn with $\psi_{+3/2}$ having the energy ε_0^+ . An external magnetic field applied perpendicular to the QW plane would cause Zeeman splitting between ε_0^+ and ε_0^- . The splitting $\Delta = \varepsilon_0^+ - \varepsilon_0^-$ may also originate from the exchange interaction of the holes with spin-polarized Mn ions. The value of Δ in this case is determined by the exchange constant and depend on the degree of Mn spin polarization. The splitting of the localized energy level leads, in turn, to the splitting of the configuration resonance. Indeed, it follows from (17) that the splitting of the configuration resonances $\tilde{\varepsilon}_0^+$ and $\tilde{\varepsilon}_0^-$ corresponding to the localized levels ε_0^+ and ε_0^- is given by

$$\tilde{\Delta} = \tilde{\varepsilon}_0^+ - \tilde{\varepsilon}_0^- = \Delta + t^2 \ln \left(1 + \frac{\tilde{\Delta}}{\tilde{\varepsilon}_0^-} \right). \quad (33)$$

Unless $\tilde{\varepsilon}_0^-$ is too close to the valence band edge the last term in Eq. (33) can be neglected and $\tilde{\Delta} \approx \Delta = \varepsilon_0^+ - \varepsilon_0^-$. The applicability of this result is limited to the case $\varepsilon_0 > \Delta$. This condition, in fact, means that neither of the split bound state levels go beyond the energy range of the 2D continuum. Our consideration will be always limited to this case. The difference in the resonances positions for the two 2D holes subbands leads to the difference in the luminescence intensity for σ^+ and σ^- polarizations if one takes into account the energy distribution functions for the holes and electrons (24).

Let I^+ , I^- be the integral luminescence intensities for the circular polarizations σ^+ and σ^- , respectively. Assuming $|I^\pm - I_0| \ll I_0$ the integral polarization degree is given by

$$P = \frac{I^+ - I^-}{2I_0}.$$

With use of Eq. (31) this yields

$$P = \frac{n\pi\hbar^2}{m_{hh'}} \frac{f(\tilde{\varepsilon}_0^-) - f(\tilde{\varepsilon}_0^+) + \int_0^\infty \left[\frac{t^2(E)f(E)}{\pi^2 t^4(E) + (E - \tilde{\varepsilon}_0^+)^2} - \frac{t^2(E)f(E)}{\pi^2 t^4(E) + (E - \tilde{\varepsilon}_0^-)^2} \right] dE}{\int_0^\infty f(E) dE}. \quad (34)$$

The slow varying functions in the upper integrals can be replaced by their values 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 expanding over t^2 gives for the first-order term:

$$P = \frac{n\pi\hbar^2 t^2}{m'_{hh}} \frac{f(\tilde{\varepsilon}_0^-)(\tilde{\varepsilon}_0^-)^{-1} - f(\tilde{\varepsilon}_0^+)(\tilde{\varepsilon}_0^+)^{-1}}{\int_0^\infty f(E) dE}. \quad (35)$$

The formula (35) leaves not much room for further simplification for the general case of $f_e(E), f_h(E)$ being two arbitrary Fermi distributions characterized by the chemical potentials μ_e, μ_h and the temperatures T_e and T_h , respectively. Let us analyze a few particular cases leading to compact analytical expressions for P . All the cases imply $\tilde{\varepsilon}_0 > \Delta$. Firstly, let the holes be fully degenerate and both energies $\tilde{\varepsilon}_0^-$ and $\tilde{\varepsilon}_0^+$ lying well beyond the quasi-Fermi level of the holes so that $\mu_h - \tilde{\varepsilon}_0^+ \gg \Delta$. In this case the distribution function of the holes can be considered as $F_h(E) = 1$ in the range $E \in (\tilde{\varepsilon}_0^-, \tilde{\varepsilon}_0^+)$. Assuming further the electrons to be nondegenerate the formula (35) is reduced to

$$P = P_1 e^{-\frac{\tilde{\varepsilon}_0}{kT^*}} \sinh \frac{\Delta}{2kT^*}, \quad (36)$$

where

$$P_1 = \frac{2\pi n\hbar^2 t^2}{m'_{hh} \tilde{\varepsilon}_0 kT^*}.$$

Here $T^* = \alpha T_e$. Exactly the same expression is valid for the case when both electrons and holes are nondegenerate. The only difference from the previously considered case is that now the effective temperature T^* is given by

$$\frac{1}{T^*} = \left(\frac{1}{\alpha T_e} + \frac{1}{T} \right).$$

The expression (36) is plotted in Fig. 3 for different values of the parameter $\gamma \equiv \Delta/\tilde{\varepsilon}_0$. The polarization shows non-monotonous behavior with increasing the temperature. In the discussed theory the polarization arises from splitting of the configuration resonance positions for σ^+ and σ^- spectra. The configuration resonance itself causes the redistribution of the transition rate in the vicinity of the resonance energy conserving the total rate, thus the net polarization is subject to the difference in occupation numbers for $\tilde{\varepsilon}_0^-$ and $\tilde{\varepsilon}_0^+$. The maximum integral polarization is therefore naturally expected when the derivative of the combined distribution function $f(E)$ reaches its maximum within the range $E \in (\tilde{\varepsilon}_0^-, \tilde{\varepsilon}_0^+)$. For the considered nondegenerate energy distribution function the maximum of the derivative is at $\tilde{\varepsilon}_0$ when $\tilde{\varepsilon}_0 = kT^*$ and the value of the derivative decreases with increase of $\tilde{\varepsilon}_0$. This explains the overall decrease of the maximum polarization with decrease of γ in Fig. 3.

For another case we consider the electron distribution function f_e being nearly constant within the configuration resonances. This can be due to the electron nonequilibrium distribution with a high quasi-Fermi level or high electron temperature T_e . The holes are now considered to have a Fermi distribution function characterized by the chemical potential μ_h and the temperature T . We also assume $kT \ll \tilde{\varepsilon}_0$. In this case from (35) we get

$$P = P_0 \left(\frac{2 \exp(\beta\xi) \sinh(\xi/2) + \gamma}{\exp(2\beta\xi) + 2 \exp(\beta\xi) \cosh(\xi/2) + 1} \right), \quad (37)$$

where

$$\beta = \frac{\tilde{\varepsilon}_0 - \mu_h}{\Delta}, \quad \xi = \Delta/kT, \quad P_0 = \frac{n\pi\hbar^2 t^2}{m'_{hh} \mu_h^2}. \quad (38)$$

The dependence (37) of P/P_0 on $1/\xi$ is plotted in Fig. 4 for different values of the parameter β (the value of γ was taken 0.1). In this case the maximum of the distribution function derivative is at the holes' Fermi level μ_h , therefore the largest integral polarization corresponds to $\beta = 0$. For this particular case (37) simplifies into

$$P = P_0 \left(\tanh(\xi) + \frac{\gamma}{2 \cosh^2(\xi)} \right). \quad (39)$$

The calculated integral polarization can be alternatively expressed through an effective g factor of the holes g_{eff} . Let us consider the Zeeman term in the Hamiltonian of the 2D holes:

$$H_B = \mu_0 g_{\text{eff}} J_z B,$$

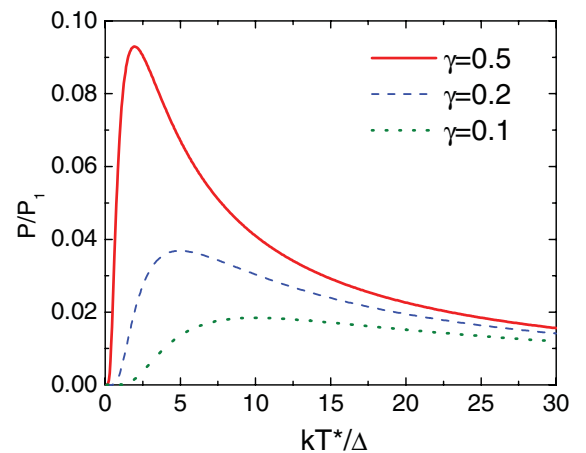


FIG. 3. (Color online) Temperature dependence of integral polarization. Electrons are nondegenerate; holes are either nondegenerate or have the constant distribution function for different values of parameter $\gamma \equiv \Delta/\tilde{\varepsilon}_0$.

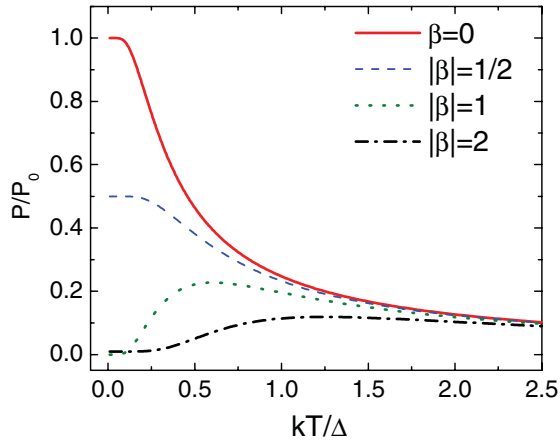


FIG. 4. (Color online) Temperature dependence of polarization for the case of electron distribution function being constant within the configuration resonances. The parameter $\beta \equiv \frac{\tilde{\varepsilon}_0 - \mu_h}{\Delta}$ denotes deviation of the holes Fermi level from the configuration resonance $\gamma = 0.1$.

where J_z is the angular momentum projection operator, μ_0 is the Bohr magneton, and B is the magnetic field applied along the z direction. The polarization of 2D holes due to the splitting between the two subbands with $j = +3/2$ and $j = -3/2$ is given by

$$P_B = \frac{\int_0^\infty (f(E - \Delta_B/2) - f(E + \Delta_B/2))dE}{\int_0^\infty (f(E - \Delta_B/2) + f(E + \Delta_B/2))dE}, \quad (40)$$

where $\Delta_B = 3\mu_0 g_{\text{eff}} B$. For the nondegenerate case one gets

$$P_B = \tanh \frac{\Delta_B}{2kT^*}. \quad (41)$$

Comparing Eq. (41) with Eq. (36) gives

$$g_{\text{eff}} = \frac{2kT^*}{3\mu_0 B} \tanh^{-1} \left[\left(\frac{2\pi n \hbar^2 t^2}{m_{hh} \tilde{\varepsilon}_0 kT^*} \right) e^{-\frac{\tilde{\varepsilon}_0}{kT^*}} \sinh \frac{\Delta_B}{2kT^*} \right]. \quad (42)$$

In the same way an expression for the degenerate case can be easily obtained.

V. DISCUSSION

The key advantage of the Fano approach used in the present study is that the unknown eigenfunctions of the complex system are expressed through the known ones of the uncoupled states; in our case these are the hole localized at Mn and the free 2D hole in the QW. Given the expansion (9) any effects on the localized state can be translated into effects for the whole coupled system. The binding energy for a hole at a single Mn in GaAs is known to be $E_0 \approx 110$ meV.¹⁴ For the enhanced Mn concentrations in the delta layer up to 10^{13} cm⁻² the impurity band is established with the binding energy lowering down to 50 meV or even less.¹⁵⁻¹⁷ In this case for the valence band QW depth starting from 50 meV the considered resonance tunneling effects are expected. Estimations for the splitting energy Δ subject to both exchange interaction between the hole and Mn and the external magnetic field. For small concentration of Mn the Zeeman splitting can be simply estimated as $\Delta = \mu_0 g B$ with B being an external magnetic field and $g \approx 3$ is the g factor for the hole at Mn.

This makes $\Delta \sim 0.1$ meV for $B \sim 1$ T. Samples with higher Mn concentrations up to a few percent are known to exhibit ferromagnetic properties;¹⁶ in this case the levels splitting Δ is to be considered with account for p - d exchange interaction.¹⁶ The particular value of Δ for typical experimental samples still remains questionable; in the ferromagnetic regime the splitting is believed to be in the range $\Delta \sim 1 - 10$ meV by the order of magnitude. The magnitude of the tunnel coupling is, of course, the key parameter determining the polarization. From Eqs. (8) and (14) it follows that the tunneling parameter can be estimated as

$$t^2 = \left(\frac{\hbar^2}{2m_0} \right)^2 \frac{2m_{hh} m'_{hh} E_0}{\hbar^4} e^{-2\sqrt{\frac{2m_{hh} E_0}{\hbar}} d}. \quad (43)$$

Substituting $E_0 = 100$ meV, $d = 4$ nm one obtains the characteristic value $t^2 \sim 0.1$ meV. We then take the Mn concentration $n \sim 10^{12}$ cm⁻², $\xi = 1$, $\varepsilon_0 \sim 3$ meV, $\beta = 0$. This set of parameters gives an estimate for the integral polarization degree $P_0 \approx 0.2$, $P_1 \approx 0.6$. The experimental temperature dependence of polarization obtained in Ref. 10 qualitatively agrees with (39). Beside the analytical expressions for the general case (35) and particular cases (36) and (39), a numerical simulation of the PL spectra can be performed based on (30) with account for the inhomogeneous broadening. An example of such calculation is shown in Fig. 5. For the calculation the following parameters were taken: $\Delta = 1$ meV, $n = 10^{11}$ cm⁻², $T = T_e = 20$ K, and $\varepsilon_0 = \mu_h = 1$ meV; the inhomogeneous broadening of the spectra was accounted for by normal distribution of E_g with the dispersion $\sigma = 3$ meV (corresponds to the fluctuation of the QW width by half a monolayer). The calculated spectra presented in Fig. 5 seem to be in good agreement with the experimental results obtained in Refs. 9 and 10. The energy shift of the spectra peaks appears to be ≈ 0.2 meV being substantially less than Δ . It is worth noting that in our theory the polarization originates from the splitting of the bound hole state at Mn and therefore may exceed the polarization degree expected from an intrinsic g factor of the 2D holes located in the QW

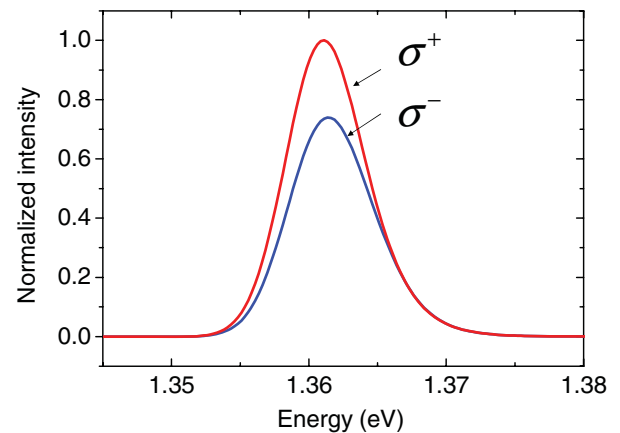


FIG. 5. (Color online) An example of calculated luminescence spectra for right (σ^+) and left (σ^-) circular polarizations with account of inhomogeneous broadening. The parameters used in calculations are given in the text. The energy shift of the peaks is ≈ 0.2 meV.

(this polarization is also of the opposite sign). However, it clearly reveals itself in the photoluminescence spectra in the wavelength range corresponding to the QW bandgap. As seen from (35) the degree of such polarization is governed by the concentration of the impurities and the value of localized level splitting which can be caused either by Zeeman effect or by exchange interaction of the localized hole with Mn *d*-electron states.

As mentioned in Sec. II the external magnetic field was assumed nonquantizing. Indeed an estimate for the energy of Landau levels separation gives

$$\hbar\omega_c = \frac{e\hbar B}{m'_{hh}c} \approx 0.3 \text{ meV}$$

for the magnetic field $B = 0.5$ T. This value is substantially less than the typical kinetic energy of the holes estimated as $\varepsilon \approx 1\text{--}10$ meV. However, this value is comparable with the tunneling parameter t^2 . Therefore for the experimental data the validity of the developed theory is well justified for $B \lesssim 0.5$ T.

VI. SUMMARY

The presented theory treats the configuration interaction between a continuum of states in the QW and a paramagnetic impurity 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

bound impurity states always leads to the enhancement of the luminescence spectral density at the configuration resonance. This new result is not covered by the conventional Fano formula.^{1,2} The redistribution of the PL spectral density in the vicinity of the resonance does not affect the integral intensity but it causes 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 presented theory expresses the eigenstates of the system with weak tunnel coupling through the wave functions of the hole localized at the paramagnetic center and the 2D states of the continuum. For this reason it seems to be 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 localized hole states provided by the free 2D carriers located at a tunnel distance.

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