Spin polaron and bistability in ferromagnetic semiconductor quantum structures

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This work shows that the in-plane localization of a hole confined in a ferromagnetic semiconductor quantum well (QW) can lead to significant energy gain if spontaneous easy-plane magnetization is mediated by the mechanisms other than itinerant carriers. The hole spin normal to the QW plane reorients the in-plane magnetization of the ferromagnetic layer at the location of polaron formation, resulting in an exchange potential with a discrete level of localization. A flexible model that incorporates the magnetization gradient term, as well as magnetic anisotropy, is proposed. In contrast to the calculations of magnetic polaron in the paramagnetic semiconductors, the energy of spin polaron in a ferromagnetic semiconductor is almost independent of the temperature in a wide range below the critical temperature of phase transition. Our calculation also demonstrates the existence of bistability in the hole state when the structure consists of appropriate ferromagnetic and nonmagnetic QWs separated by a finite barrier. Hence, a memory element that can be scaled down to a single hole may be achieved through polaron formation.

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I. INTRODUCTION

Recently, much attention has been directed to achieve diluted magnetic semiconductors (DMSs) with a high Curie temperature. In the most extensively studied case of $A^3_{1-x}Mn_xB^5$ compounds, the Mn doping leads to mutual ordering of hole and magnetic ion spins, which is the most probable mechanism for ferromagnetism in such semiconductors.[1] However, the carrier-mediated ferromagnetism[2] is not the only mechanism available in the DMSs. The sign of interion exchange interaction can take a positive value (depending on the electronic structure of the magnetic ion) that results in ferromagnetism without itinerant carriers. An example of this type can be found in Cr-based DMSs with a ferromagnetic superexchange interaction. Besides, the indirect spin-spin interaction via virtual carriers (the Blombergen-Rouland mechanism) could also be responsible for ferromagnetic (FM) semiconductor formation. Note that laser excitation with the sub-bandgap energy further enhances this effect.[3,4]

When in the FM state with spontaneous magnetization, the electronic state of a DMS is affected by strong exchange interaction with the spin-polarized magnetic ions resulting in a giant spin splitting in the energy bands; on the other hand, no such splitting is expected in the paramagnetic phase. Moreover, spontaneous magnetization in the FM DMS leads to suppression of the longitudinal magnetic susceptibility $\chi_{\|}$ at low-enough temperatures. Hence, any effects relying on some additional magnetization in the longitudinal direction become very difficult to realize in the FM semiconductors. This is the reason why the spin polaron, which is a self-consistent trapping of an electron (or a hole) by the effective exchange potential of magnetic ions, has been explored only in paramagnetic semiconductors. With their spin directed along that of magnetic ions, the electrons cannot sufficiently alter the local polarization in a FM DMS.

This work draws attention to a different type of polaron formation in a DMS quantum well (QW) whose FM phase is mediated by the mechanisms independent of the presence of itinerant carriers (see the discussion above). Specifically, we consider the case of a heavy hole (HH) confined in a QW (Ref. 5) with the hole effective field normal to the QW plane,[6] while the vector of spontaneous magnetization lies in the plane of the QW perpendicular (instead of parallel) to the hole spin. The corresponding in-plane effective field does not split the hole state substantially due to a large heavy hole g-factor anisotropy.[7] Meanwhile, if lateral HH localization can be introduced, the finite hole effective field that is normal to the QW plane shifts the magnetization vector away from the QW plane as shown schematically in Fig. 1. The amount of deviation is proportional to the transversal FM susceptibility $\chi_{\perp}$, which, in general, exceeds $\chi_{\|}$ significantly. (A similar modification in Mn in-plane magnetization was observed when spin-polarized HHs were injected optically in GaMnAs.[8]) The normal component of the FM layer magnetization that arises in the vicinity of the localized hole plays the role of a self-consistent potential and subsequently traps the hole with discrete energy levels; in other words, it forms a (localized) polaron state. Clearly, there are other phenomena, such as interion exchange interaction and magnetic an-

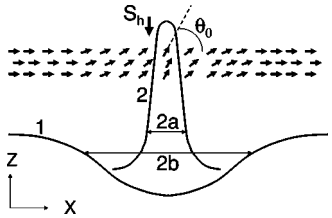

FIG. 1. Schematic diagram of polaron formation in a FM QW; $\hat{x}$ and $\hat{z}$ are the directions of easy magnetization and normal to the QW plane. Small arrows show the local magnetization direction of the FM layer and θ_0 the maximal angle of its deviation. Curves 1 and 2 depict the in-plane effective magnetic potential well and the hole wave function after polaron formation. The hole spin $\vec{S}_h$ can be either parallel or antiparallel to the z axis. Only one case is considered as they are equivalent.

isotropy, that hamper this effect. Hence, a quantitative analysis of the conditions for hole-polaron formation in a FM QW is the primary aim of our investigation. Note that *n*-type DMSs can reveal FM properties;[9] however, electrons cannot form a noncollinear configuration with the vector of spontaneous magnetization due to the very small electron spin-orbital interaction.

II. THEORETICAL MODEL

To be specific, let us consider a thin FM QW with the *x*-*y* plane of easy magnetization. For simplicity, the *z* axis is chosen as the QW growth direction while the magnetization vector $\vec{M}_0$ is along the *x* axis. Localization of a hole in the QW with the wave function $\psi(\vec{r})$ leads to a change in the magnetization vector $\vec{M}=\vec{M}_0+\Delta\vec{M}$ from the QW plane due to the effective exchange field as mentioned above. The total free energy *F* of a localized hole and the magnetic energy modified by this localization may be described under a continuum approximation of the magnetic medium. This treatment neglects the compositional fluctuations and considers the magnetic properties as a function of local magnetization $\vec{M}=\vec{M}(\vec{r})$. Then, the free-energy contribution ΔF associated with the hole localization in the FM semiconductor can be expressed as

$$\Delta F = T + U_{QW} + V_{int}(\Delta\vec{M}) + A(\vec{\nabla}\vec{M}) + K(\Delta\vec{M}) + D(\Delta\vec{M}). \tag{1}$$

Here, the kinetic energy of the localized hole in the one-band approximation assumes the form $T=T_x+T_y+T_z$ with

$$T_i = -\frac{\hbar^2}{2m_i}\langle\psi|\nabla_i^2|\psi\rangle, \tag{2}$$

where $i=x,y,z$; m_z and $m_x=m_y$ are the effective masses along the QW growth and in-plane directions. An earlier analysis of magnetic polarons in DMS QWs illustrated the crucial influence of slight in-plane hole localization caused by the interfaces roughness on polaron formation.[10] In a gated structure, similar localization can be realized by an electrical bias. Therefore, we take the corresponding lateral potential $u(x,y)$ into consideration of the confinement energy U_{QW} along with the QW potential U_0

$$U_{QW} = \langle\psi|U_0(z) + u(x,y)|\psi\rangle. \tag{3}$$

The third term in Eq. (1) represents the energy of the localized hole-exchange interaction with magnetic ions of the FM layer. It can be written in terms of local magnetization as[11–13]

$$V_{int} = \langle\psi|\frac{1}{2}\beta n_m S\frac{\Delta\vec{M}(\vec{r})\hat{z}}{M_{sat}}|\psi\rangle, \tag{4}$$

where β is an integral of hole-ion exchange interaction, n_m the concentration of magnetic ions, *S* the spin of the magnetic ion, and M_{sat} the saturation value of the FM magnetization. This equation accounts for the magnetic energy of the FM QW in the effective field (in units of energy) of a localized hole $\vec{h}=\pm\frac{1}{2}\hat{z}\beta|\psi|^2$ located in the state with the *z* projection of spin $\frac{1}{2}$ or $-\frac{1}{2}$. Thermal fluctuations between these states can reduce the $\vec{h}$ strength by a factor $r_T=\exp(-E_{pol}/T)$, where E_{pol} is the polaron energy.[14] Hence, $r_T \ll 1$ is considered hereinafter.

In the one-band model, the hole wave function $\psi(\vec{r})$ is a HH state with the effective spin directed along the *z* axis. This approximation is adequate for the polaron wave function in zinc-blend semiconductors (e.g., see Ref. 15) if T_x, $T_y \ll \Delta E_{HL}$ (ΔE_{HL} is the HH–light hole splitting).[16] For a more precise analysis, a 4×4 Luttinger Hamiltonian[17,18] can be used. When the exchange interaction of magnetic ions with the *x* and *y* components of hole spin is taken into account, the resulting hole spin deviates from the *z* direction. The contribution of this effect to the total energy was estimated as[19] $G_{x\text{-}y}^3/\Delta E_{HL}^2$ ($G_{x\text{-}y}$ is the in-plane component of the magnetic ion effective magnetic field in units of energy). At the same time, lateral hole localization can induce the in-plane spin component. For simplicity of the analysis, we assume that the present case satisfies the conditions for the one-band treatment as discussed above (for example, weak in-plane hole confinement, etc.).

The first three terms of Eq. (1) coincide with those for the magnetic polaron in paramagnetic semiconductors. In the latter case, the actual dependence of $\vec{M}$ on the hole effective field $h(\vec{r})$ (i.e., $|\vec{M}|\to M_{sat}$ as $h\to\infty$) allows one to reduce the problem to minimization of a nonlinear Hamiltonian by using a trial function ψ.[12,13] However, the case under consideration is more complicated due to the additional contribution of specific FM terms to the ΔF that results in a nonlocal effective hole potential. For simplicity, our model takes into account only the rotation of $\vec{M}=\vec{m}M_0$ ($M_0=|\vec{M}|$) that does not change the quantity of microscopic states of the system. It means that the entropy part of the free energy does not change when polaron formation occur in the FM layer. As a result, the temperature dependence of this process will be defined via the temperature dependence of the parameters involved in the model and not via the entropy part.

The remaining three terms in Eq. (1) are the most important energy terms of a ferromagnet, which describe such phenomena as FM resonance[20] or magnetic domain wall structure.[21] The first two terms (of the last three) describe the contribution of inhomogeneous magnetization to the exchange energy (*A*) and to the energy of in-plane anisotropy (*K*) with respect to the direction $\vec{\sigma}=\hat{x}$

$$A = \frac{\alpha}{2}\int\sum_{i,j}\left(\frac{\partial m_j}{\partial x_i}\right)^2 d^3\vec{r}; \tag{5}$$

$$K = \varkappa\int[1-(\vec{m}\vec{\sigma})^2]d^3\vec{r}. \tag{6}$$

Equation (5) tends to widen the polaron area, while the anisotropy [Eq. (6)] works for squeezing the polaron size. An order-of-magnitude estimate shows $\alpha\sim k_B T_c n_m^{1/3}$, while $\varkappa$ is determined by the spin-orbital interaction and the low-symmetry potential (or crystal structure), which constitute the easy-plane magnetization. Practically, both α and $\varkappa$ can be deduced from appropriate experiments. The last term *D* is

the magnetic energy in a demagnetization field that depends on the size and shape of a magnet. However, this field is negligible in the limit of thin but wide magnetic film. Thus, it is neglected from further consideration.

As mentioned above, the desired solution can be obtained by finding the hole wave function $\psi(\vec{r})$ that minimizes the free energy given in Eq. (1). As a trial wave function, we adopt

$$\psi(\vec{r}) = \psi_1(z)\sqrt{\frac{2}{\pi a^2}}e^{-\rho^2/a^2}, \tag{7}$$

where $\psi_1(z)$ corresponds to hole confinement in the QW, $\rho = \sqrt{x^2+y^2}$, and a is the radius of polaron localization in the QW plane that is used as an optimization parameter in the variational procedure. Once $\psi(\vec{r})$ is calculated, the magnetization $\vec{M}$ can be found as the solution of a magnetostatic problem with an effective field $\vec{h}$ that constitutes the self-consistent potential for in-plane hole localization. This problem can also be considered in terms of a variational procedure with the approximation

$$\vec{m} = \{\cos\theta, 0, \sin\theta\};\ \theta = \theta_0 e^{-\rho^2/b^2}. \tag{8}$$

According to the definition, $\theta = \theta(\rho)$ is the angle of local magnetization deviation from the direction $\vec{\sigma} = (1,0,0)$; the variational parameters θ_0 and b represent the maximal angle θ and the radius of magnetic potential well when the spin polaron is formed (see Fig. 1).

Now we can calculate all components of the free energy [Eq. (1)] in terms of parameters a, b, and θ_0. In doing so, we rewrite Eq. (1) in terms of energy unit $U_s = \frac{1}{2}|\beta| n_m S'$ ($S' = SM_0/M_{sat}$) and length unit $d_s = \hbar/\sqrt{2mU_s}$ (see Refs. 11–13). After some algebra, we come to the trial functional in the form

$$\Delta F = \frac{1}{a^2} - u_{loc}(1 - e^{-r_0/a}) - \int_0^\infty e^{-x}\sin(\theta_0 e^{-\gamma x})dx + \alpha_s\theta_0^2 + \varkappa_s b^2 \int_0^\infty [1 - \cos^2(\theta_0 e^{-x})]dx. \tag{9}$$

To obtain the second term, we use a simple approximation[22] $u(x,y) = u(\rho) = -u_{loc}$ if $\rho < r_0$, and $u(\rho) = 0$ if $\rho > r_0$, where u_{loc} is the depth of the lateral (nonmagnetic) potential well with the radius r_0. Other notifications in Eq. (9) are $\gamma = a^2/2b^2$, $\alpha_s = \pi\alpha L_w/|\beta| n_m S'$, and $\varkappa_s = 2\pi\varkappa L_w d_s^2/|\beta| n_m S'$ with the FM QW width L_w. The minimum of ΔF with respect to a, θ_0, and b gives the polaron state as a function of parameters u_{loc}, r_0, α_s, and $\varkappa_s$.

III. RESULTS AND DISCUSSION

Apparently, the minimization procedure of the trial function [Eq. (9)] can be fulfilled only numerically. Doing this requires an estimation of U_s, d_s, u_{loc}, r_0, α_s, and $\varkappa_s$ in terms of typical values of DMS band parameters. We choose $\beta\Omega_0^{-1} = -1.2$ eV, the primitive unit cell volume $\Omega_0 = 55$ Å^3, the magnetic ion content $x = 0.1$, and $m = 0.3m_0$ (m_0 is the free-electron mass), and assume $S' = 0.8S$, $S = 5/2$ that defines the energy and length units $U_s = k_B \times 1400$ K (k_B is the Boltzmann constant) and $d_s = 10$ Å. Parameters α and $\varkappa$ in Eqs. (5) and (6) are taken from the experiments.[23] By using a notation $L_w = \lambda \times 100$ Å, one can find $\alpha_s = 0.52\lambda$ and $\varkappa_s = 7 \times 10^{-5}\lambda$.

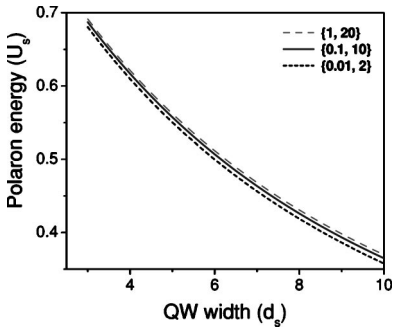

FIG. 2. Polaron energy E_{pol} as a function of QW width L_w for lateral potential parameters $\{u_{loc}, r_0\} = \{0.01, 2\}$, $\{0.1, 10\}$, $\{1, 20\}$ in units of U_s and d_s. The other parameters of the FM QW are as discussed in the text.

Figure 2 illustrates the polaron energy as a function of QW width L_w. The polaron energy is calculated as

$$E_{pol} = \Delta F - E_{NM}, \tag{10}$$

where the nonmagnetic energy E_{NM} associated with in-plane hole localization [i.e., the first two terms of Eq. (2)] is subtracted from ΔF. The numerical calculations are carried out with three sets of lateral potential parameters $\{u_{loc}, r_0\} = \{0.01, 2\}, \{0.1, 10\}, \{1, 20\}$ (in units of U_s and d_s). The potential $u(x,y)$ with $\{u_{loc}, r_0\} = \{0.01, 2\}$ corresponds to that estimated in the II-VI compounds for roughness induced localization,[22] while the others are the conditions one can expect in a gated structure with appropriate biases. As can be seen from the figure, the results for these three cases are nearly identical; accordingly, the polaron energy seems to be rather insensitive to the nature of in-plane localization prior to polaron formation. A similar finding was made in the II-VI paramagnetic QWs earlier, where the so-called selective excitation method is just based on the polaron energy independence of the "prelocalization" potential.[10] Figure 2 also illustrates that narrow FM QWs are more favorable to reach the maximum polaron effect.

A possible application of polaron state might stem from its bistability in a quantum structure with both magnetic and nonmagnetic (NM) layers. Note that the most extensively studied structure for polaron bistability is a NM QW embedded in the DMS barriers. In this case, hole localization near any one interface can be more favorable than that in the QW centrum due to the nonlinear nature of the hole exchange interaction with the DMS barriers.[13,24] In the present study, we envision a structure that consists of a FM QW and a NM QW separated by a NM barrier of finite height (see Fig. 3). It is also assumed that the potential profile of the structure can be engineered so that the bottom of the FM QW (without the exchange interaction) is somewhat higher (by ΔU) than the bottom of the NM QW as in Fig. 3(a). Subsequently, the hole

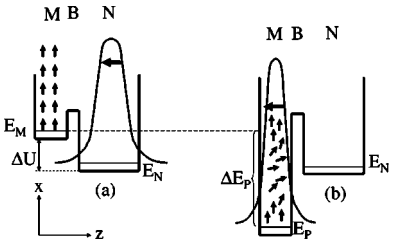

FIG. 3. Bistability with respect to hole localization (a) in the NM QW (N) or (b) in the FM QW (M) with polaron formation. A nonmagnetic barrier (B) separates the NM and FM QWs; E_N and $E_M(E_P)$ are the eigenenergies of hole localization in the NM QW and the FM QW without (with) polaron formation, respectively; and ΔE_P is the energy of polaron formation. Curves depict the hole ψ function in the NM and FM QWs. Small arrows indicate the local magnetization directions; the large arrow is the hole spin directed normal to the QW plane. It is important to note that the device does not require a polarized hole gas in the NM QW. Once a hole is injected into the FM QW with the spin directed either parallel or antiparallel to the growth direction (a 50-50 split in the unpolarized gas), it provides an effective field normal to the QW plane. Only one case is shown schematically for simplicity as in Fig. 1.

ground state is almost wholly localized in the NM QW with an energy E_N, while a small penetration into the FM QW (due to the tail of the wave function) is not enough to form a polaron. However, the polaron state E_P of the hole localized in the FM QW can be deeper than E_N if the effective hole exchange potential stemmed from $V_{int}(\Delta\vec{M})$ exceeds the sum of ΔU and other energy losses associated with hole localization. This case corresponds to the polaron ground state [Fig. 3(b)]. Thus, the structure described above can realize two stable hole states under the same external conditions. Note that multistability can be reached due to separation of the carrier spins in a digital FM heterostructure.[25] However, two coupled QWs, FM and NM, give more possibilities to detect the system in any one of the stable states.

To quantitatively describe the hole bistability, let us assume that the z component of the hole wave function can be expressed as a combination of the individual states $\psi_M(z)$ and $\psi_N(z)$ obtained in each (FM or NM) QW

$$\psi_1(z) = c_M\psi_M(z) + c_N\psi_N(z), \tag{11}$$

where $|c_M|^2$ ($|c_N|^2$) is the hole-localization probability in the FM (NM) QW, respectively. If the overlap between $\psi_M(z)$ and $\psi_N(z)$ is not significant, then the total free energy of the structure can be written as a sum

$$\Delta F_{2W} = \cos^2\varphi[T + U_{QW} + V_{int}(\Delta\vec{M})] + A(\vec{\nabla}\vec{M}) + K(\Delta\vec{M}) + \sin^2\varphi E_N, \tag{12}$$

where the parameter φ is defined according to the equations $\cos^2\varphi = |c_M|^2$, $\sin^2\varphi = |cN|^2$. The case with a small or negative ΔU suits a single minimum of ΔF_{2W} at $\varphi = 0$ (i.e., the FM QW), while $\varphi = \pi/2$ provides the maximum. Any deviation of φ from $\pi/2$ tends the hole to the polaron ground state in the FM QW. A similar situation is expected for a large positive ΔU when the polaron state with $\varphi = 0$ becomes unstable

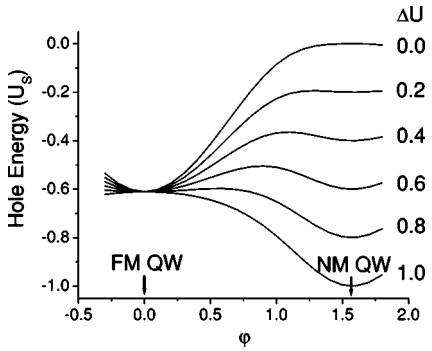

FIG. 4. Dependence of hole energy ΔF_{2W} as a function of φ and E_N. $\cos^2\varphi(\sin^2\varphi)$ is a probability of hole localization in the FM QW (NM QW). The energy scale is in units of U_s assuming $E_M = 0$. ΔU is as defined in Fig. 3. The calculation is conducted for $L_w = 50$ Å and $\{u_{\rm loc}, r_0\} = \{0.1, 10\}$; the other parameters are the same as in Fig. 2. The bistability is observed for ΔU in the range 0.2–0.8.

while localization in the NM QW corresponds to the ground state. The calculation in Fig. 4 shows that the desired bistable states (with two local minima near $\varphi = 0$ and $\varphi = \pi/2$) can be achieved, if ΔU is in the range between 0.2 and 0.8 (in units of U_s) with a proper choice of NM and FM band parameters. In such a case, a small deviation from the local minima will not disturb the system (i.e., *stable*). Moreover, the relative values of E_N can be controlled externally (e.g., by a gate bias pulse) enabling hole transfer between the two stable states, each localized in the NM QW or the FM QW. This is a desired feature of a memory device.

IV. SUMMARY

In this paper, we demonstrated the possibility of polaron formation in the FM QWs provided in-plane spontaneous magnetization arises due to direct (rather than indirect via itinerant carriers) magnetic ion spin-spin interaction. Hole localization results in an appearance of an effective magnetic field directed along the QW growth direction that, in turn, modifies locally the magnetization vector. The exchange interaction with the reoriented magnetization provides a stable hole spin-polaron state. We proposed a model that describes this phenomenon based on an assumption of (nearly) saturated magnetization in the FM QW. Moreover, our results show that a hole can exhibit stable localization in the FM QW or the NM QW under the same external conditions, if polaron formation is taken into account. The transition from one of the bistable states to the other through the monostable states (in the FM or NM QWs) can be achieved by controlling the interwell energy separation through a gate bias pulse. This opens an opportunity for realizing a memory cell device that can be scaled down to a single hole.

ACKNOWLEDGMENTS

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