Magnetic impurity in a quantum well of a IV–VI narrow-gap semiconductor

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Abstract. We study the magnetic density distribution created by a separate magnetic impurity placed inside a IV–VI semiconductor quantum well. The absence of carriers is assumed, so that the induced magnetic density is due to virtual electron–hole excitations. The origin of this effect is analogous to the vacuum screening of charge in quantum electrodynamics. We calculate the magnetic density for different positions of the impurity within the well. The interaction between magnetic impurities in the quantum well is also calculated.

The investigation of magnetic impurities in quantum wells (QW) is of interest because spectrum quantization gives rise to a change in both the wavefunctions and the coupling to impurities as compared to three-dimensional crystals. As a result, the magnetic impurity interaction becomes dependent on the geometric parameters of the QW and the position of the impurity inside the well.

In the present paper we study a separate magnetic impurity within a QW. We calculate the spatial distribution of magnetic density created by impurity spin. In our treatment we assume the filling of quantized levels to be absent (or the chemical potential to be in the middle of the gap) so that the distribution of magnetic density arising in the QW is an effect of vacuum screening of the impurity spin analogous to the known effect of vacuum screening of charge in quantum electrodynamics [1].

There are some problems about calculating the electronic properties of IV–VI semiconducting QWs due to the complicated energy spectrum of two-dimensional carriers in these systems [2–5]. We are going to use a model of the spectrum proposed in [5], which is convenient for the description of low-energy electron–hole excitations. This model is exact in the case of infinitely high energy walls.

Restricting ourselves to take account of only one pair of the nearest electron–hole levels, the Hamiltonian of 2D carriers reads as [5]

$$\mathcal{H}_0 = \begin{pmatrix} \varepsilon_0 \sigma_z + v \sigma \cdot \mathbf{k} & 0 \\ 0 & -\varepsilon_0 \sigma_z + v \sigma \cdot \mathbf{k} \end{pmatrix} \quad (1)$$

where $2\varepsilon_0$ is the energy gap ($\varepsilon_0, -\varepsilon_0$ is the pair of closest size-quantized levels), $\mathbf{k}$ is the two-dimensional wavevector in the QW plane, σ are the Pauli matrices and the z axis is chosen perpendicular to the QW plane. The basis

wavefunctions for the matrix $\mathcal{H}_0$ are a set of functions $|c \uparrow\rangle, |v \downarrow\rangle, |v \uparrow\rangle, |c \downarrow\rangle$ corresponding to quantized levels for $\mathbf{k} = 0$ with certain spin orientations, multiplied by $\exp(i\mathbf{k} \cdot \mathbf{r})$. Note that the Hamiltonian (1) is isotropic, and does not contain any second-order terms in $\mathbf{k}$. We will discuss it later.

The interaction with the magnetic impurity $S(\mathbf{x})$ is taken in the form

$$\mathcal{H}_{\text{int}} = J \int d^2x S(\mathbf{x}) \cdot \gamma \quad (2)$$

where matrices γ consist of the matrix elements of s – d interaction with the basis wavefunctions of Hamiltonian (1), $S(\mathbf{x})$ is the ‘bare’ magnetic density and J is the coupling constant.

This is the simplest form of interaction with only one coupling constant J . In fact, such a form can be accepted only as a model, since the real magnetic impurity could be described by a matrix γ with a number of different constants.

The basis wavefunctions have been presented in an explicit form in [5]. They include the symmetric and asymmetric functions with respect to reflection in the QW plane. Therefore, in the calculation of matrices γ , the position of an impurity inside the QW is important.

We can present the impurity potential as a superposition of functions of opposite symmetry. Correspondingly, we can write

$$\gamma = \alpha \gamma^{(s)} + \beta \gamma^{(a)} \quad (3)$$

where $\gamma^{(s)}$ should be calculated with a symmetric potential,

and $\gamma^{(a)}$ with an asymmetric one. They are given by

$$\begin{aligned}\gamma_x^{(s)} &= \begin{pmatrix} 0 & i\sigma_y \\ -i\sigma_y & 0 \end{pmatrix} & \gamma_y^{(s)} &= \begin{pmatrix} 0 & -i\sigma_x \\ i\sigma_x & 0 \end{pmatrix} \\ \gamma_z^{(s)} &= \begin{pmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix} & \gamma_x^{(a)} &= \begin{pmatrix} \sigma_y & 0 \\ 0 & \sigma_y \end{pmatrix} \\ \gamma_y^{(a)} &= \begin{pmatrix} -\sigma_x & 0 \\ 0 & -\sigma_x \end{pmatrix} & \gamma_z^{(a)} &= \begin{pmatrix} 0 & i\sigma_z \\ -i\sigma_z & 0 \end{pmatrix}\end{aligned}\quad (4)$$

as follows from direct calculation with the aid of formulae from [5].

Let us consider the partition function as a path integral over Fermi fields

$$Z = \int \mathcal{D}\psi^+(x, t) \mathcal{D}\psi(x, t) \exp(iA) \quad (5)$$

where the action

$$\begin{aligned}A &= \int d^2x dt \left[\psi^+(x, t) \left(i \frac{\partial}{\partial t} - \mathcal{H}_0 \right) \psi(x, t) \right. \\ &\quad \left. - J S_i(x, t) \psi^+(x, t) \gamma_i \psi(x, t) \right].\end{aligned}\quad (6)$$

We can introduce now the magnetic density $\mathbf{m}(x, t)$ interacting with impurity as

$$\begin{aligned}A &= \int d^2x dt \left(\int d^2x' dt' \psi^+(x, t) G_0^{-1}(x, t, x', t') \psi(x', t') \right. \\ &\quad \left. + \lambda(x, t) \cdot [\mathbf{m}(x, t) - \psi^+(x, t) \gamma \psi(x, t)] \right. \\ &\quad \left. - J \mathbf{m}(x, t) \cdot \mathbf{S}(x, t) \right)\end{aligned}\quad (7)$$

where $G_0(x, t, x', t')$ is the Green function of free Fermi fields described by (1). Then the partition function (5) acquires the additional integration over $\mathbf{m}(x, t)$ and an auxiliary field $\lambda(x, t)$.

After that, in a standard way we can integrate out the Fermi fields ψ^+ , ψ and the auxiliary field λ . That results in

$$Z = Z_e \int \mathcal{D}\mathbf{m}(x, t) \exp(iA_m) \quad (8)$$

where Z_e is the partition function of free Fermi fields and A_m is the magnetic action

$$\begin{aligned}A_m &= \int d^2x dt \left(\frac{1}{2} \int d^2x' dt' m_i(x, t) \chi_{ij}^{-1}(x, t, x', t') m_j(x', t') \right. \\ &\quad \left. - J m_i(x, t) S_i(x, t) \right)\end{aligned}\quad (9)$$

with

$$\chi_{ij}(x, t, x', t') = -i \text{Sp} [\gamma_i G_0(x, t, x', t') \gamma_j G_0(x', t', x, t)]. \quad (10)$$

In what follows we are interested in the static magnetic impurity $\mathbf{S}(x)$. Therefore we are going to calculate the static magnetic density $\mathbf{m}(x)$. Then instead of (9) and (10) we can write

$$\begin{aligned}A_m &= \int d^2x \left(\frac{1}{2} \int d^2x' m_i(x) \chi_{ij}^{-1}(x, x') m_j(x') \right. \\ &\quad \left. - J m_i(x) S_i(x) \right)\end{aligned}\quad (11)$$

$$\chi_{ij}(x, x') = -i \text{Sp} \left(\int \frac{d\varepsilon}{2\pi} \gamma_i G_0(x, x', \varepsilon) \gamma_j G_0(x', x, \varepsilon) \right). \quad (12)$$

In accordance with (11) the susceptibility $\chi_{ij}(x, x')$ is the Green function of the equation that determines magnetic density distribution. By varying A_m over $\mathbf{m}(x)$ we obtain

$$\int d^2x' \chi_{ij}^{-1}(x, x') m_j(x') = J S_i(x). \quad (13)$$

This leads to

$$m_i(x) = J \int d^2x' \chi_{ij}(x, x') S_j(x'). \quad (14)$$

Let us consider the magnetic density arising around a point-like impurity situated at some point with $x = 0$

$$S_i(x) = S_i \delta(x). \quad (15)$$

There are several different cases:

1. If the impurity is placed in the centre of the QW, then to calculate χ_{ij} we should take for γ matrices the $\gamma^{(s)}$ from (4). Such calculations have already been performed in [6] in connection with the computation of indirect exchange interaction between magnetic impurities. Making use of χ_{ij} from [6], we can write down the final expressions for $\mathbf{m}(x, t)$ in the case of a strictly symmetrical impurity position (i.e. at the centre of the QW).

1a. If the point-like impurity has the magnetic moment directed along the z axis (perpendicular to the QW plane), then in the limits of small or large distances, the corresponding formulae are

$$m_z^{(s)}(x) = \begin{cases} -J_s S_z \frac{N_v \varepsilon_0^{1/2} \exp(-2x \varepsilon_0 / v)}{4\pi^{3/2} v^{3/2} x^{5/2}} & x \gg v/\varepsilon_0 \\ -J_s S_z \frac{N_v}{8\pi v x^3} & x \ll v/\varepsilon_0. \end{cases} \quad (16)$$

The extra factor N_v which we put in (16) is the number of valleys ($N_v = 4$ for IV–VI crystals), and the constant J_s is related to the bare coupling constant J by

$$J_s = J \int_{-\infty}^{\infty} ds \Delta(z) [\Phi_1^2(z) + \Phi_2^2(z)]. \quad (17)$$

$\Phi_1(z)$ and $\Phi_2(z)$ are symmetrical and asymmetrical functions of localized electron states in the QW [5], $\Delta(z)$ is the ‘smeared’ delta-function that is the bare z -distribution of spin density of point-like magnetic impurity†. The index s corresponds to the symmetric distribution of the magnetic density.

† It is important to distinguish between delta-functions entering (15) and (17). That is because we study the magnetic density along the QW plane $m_i(x)$, and our treatment is justified only for large distances $|x|$ (see below in discussions). On the other hand, the functions localized along the z axis are determined for $|z|$ larger than the lattice constant.

Figure 1. Coupling constants versus impurity position in a QW ($\Delta_0 = 0.01$ eV, $\varepsilon_0 = 0.04$ eV, $L = 10^{-6}$ cm).

1b. If the impurity spin is directed along the QW plane, then with the aid of [6] we obtain

$$\mathbf{m}^{(s)}(\mathbf{x}) = \begin{cases} J_s \frac{N_v \varepsilon_0^{3/2} \exp(-2x\varepsilon_0/v)}{2\pi^{3/2} v^{5/2} x^{3/2}} [\mathbf{S} - \mathbf{n}(\mathbf{n} \cdot \mathbf{S})] & x \gg v/\varepsilon_0 \\ J_s \frac{N_v}{16\pi v x^3} [\mathbf{S} - 3\mathbf{n}(\mathbf{n} \cdot \mathbf{S})] & x \ll v/\varepsilon_0 \end{cases} \quad (18)$$

where $\mathbf{n} = \mathbf{x}/|\mathbf{x}|$.

2. If the impurity is shifted from the centre of the QW to some point z_0 , the symmetric part of the magnetic density $\mathbf{m}^{(s)}(\mathbf{x})$ can be calculated in the same way as before, but instead of equation (17) one should use

$$J_s(z_0) = \frac{J}{2} \int_{-\infty}^{\infty} dz [\Delta(z - z_0) + \Delta(z + z_0)] \times [\Phi_1^2(z) + \Phi_2^2(z)]. \quad (19)$$

Let us consider the asymmetric part $\mathbf{m}^{(a)}(\mathbf{x})$. The associated coupling constant is

$$J_a(z_0) = J \int_{-\infty}^{\infty} dz \Phi_1(z) \Phi_2(z) [\Delta(z - z_0) - \Delta(z + z_0)]. \quad (20)$$

The dependences of J_s/J and J_a/J on z_0 are presented in figure 1. In this calculation we have used the following values for the parameters: $\Delta_0 = 0.01$ eV, $\varepsilon_0 = 0.04$ eV, $L = 10^{-6}$ cm and $\beta = 10^7$ cm $^{-1}$, where Δ_0 is the half-bandwidth of the semiconducting material inside the well, L is half-width of the QW and β^{-1} is the characteristic size of the impurity wavefunction. From this picture we can see that the asymmetric part of the magnetic density distribution becomes more important with increasing displacement of the impurity from the central position to the QW boundary. The susceptibility tensor χ_{ij} can be calculated with the help of (12) and matrices $\gamma_i^{(a)}$ from (4).

2a. For $\chi_{zz}(\mathbf{x}\mathbf{x}')$ components the calculations, which are completely analogous to those presented in [6], give

rise to

$$\chi_{zz}(\mathbf{x}\mathbf{x}') = -\frac{1}{\pi^3 v |\mathbf{x} - \mathbf{x}'|} \int_0^\infty d\xi (\xi^2 + \tilde{\varepsilon}_0^2) \times \left[\mathcal{K}_0^2 \left(\sqrt{\xi^2 + \tilde{\varepsilon}_0^2} \right) + \mathcal{K}_1^2 \left(\sqrt{\xi^2 + \tilde{\varepsilon}_0^2} \right) \right] \quad (21)$$

where $\mathcal{K}_v(y)$ are the Bessel functions, and $\tilde{\varepsilon}_0 = \varepsilon_0 |\mathbf{x} - \mathbf{x}'|/v$. Using (14), (18) and (21), in the limits of large and small distances we obtain

$$\mathbf{m}_z^{(a)}(\mathbf{x}) = \begin{cases} -J_a S_z \frac{N_v \varepsilon_0^{3/2} \exp(-2x\varepsilon_0/v)}{2\pi^{3/2} v^{5/2} x^{3/2}} & x \gg v/\varepsilon_0 \\ -J_a S_z \frac{N_v}{8\pi v x^3} & x \ll v/\varepsilon_0. \end{cases} \quad (22)$$

2b. The analogous calculations of longitudinal components χ_{ij} lead to

$$\chi_{ij}(\mathbf{x}\mathbf{x}') = -\frac{1}{\pi^3 v |\mathbf{x} - \mathbf{x}'|} \int_0^\infty d\xi (\xi^2 + \tilde{\varepsilon}_0^2) \times \left\{ 2n_i n_j \mathcal{K}_1^2 \left(\sqrt{\xi^2 + \tilde{\varepsilon}_0^2} \right) + \left[\mathcal{K}_0^2 \left(\sqrt{\xi^2 + \tilde{\varepsilon}_0^2} \right) - \mathcal{K}_1^2 \left(\sqrt{\xi^2 + \tilde{\varepsilon}_0^2} \right) \right] \delta_{ij} \right\} \quad (23)$$

from which follows

$$\mathbf{m}^{(a)}(\mathbf{x}) = \begin{cases} -J_a \frac{N_v \varepsilon_0^{3/2} \exp(-2x\varepsilon_0/v)}{2\pi^{3/2} v^{5/2} x^{3/2}} \mathbf{n}(\mathbf{n} \cdot \mathbf{S}) & x \gg v/\varepsilon_0 \\ J_a \frac{N_v}{16\pi v x^3} [\mathbf{S} - 3\mathbf{n}(\mathbf{n} \cdot \mathbf{S})] & x \ll v/\varepsilon_0. \end{cases} \quad (24)$$

Formulae (18) and (24) give us the symmetric and asymmetric parts of the magnetic density created by the impurity spin in the QW. The effective coupling constants J_s and J_a determined in (19) and (20) contain information about impurity position in the QW. Consequently they give us the dependence of the magnetic density on z_0 .

Thus for the arbitrary position of impurity in the QW we have the real distribution of the total density as a sum

$$\mathbf{m}(\mathbf{x}, z) = \mathbf{m}^{(s)}(\mathbf{x}) \Phi_1(z) + \mathbf{m}^{(a)}(\mathbf{x}) \Phi_2(z) \quad (25)$$

where $\mathbf{m}^{(s)}(\mathbf{x})$ is determined by (16) and (18) with $J_s = J_s(z_0)$ from (19). The vector $\mathbf{m}^{(a)}(\mathbf{x})$ is determined by (22) and (24).

The interaction between two impurities S_1 and S_2 situated at points $(0, z)$ and (x, z') is given by

$$E_{\text{int}} = \{ S_1 \cdot S_2 I_s(z, z') - (S_1 \cdot \mathbf{n})(S_2 \cdot \mathbf{n}) \times [I_s(z, z') + I_a(z, z')] F_3(x) - S_{1z} S_{2z} [I_s(z, z') F_1(x) + I_a(z, z') F_3(x)] \} \quad (26a)$$

for $x \gg v/\varepsilon_0$, and

$$E_{\text{int}} = \left\{ \frac{1}{2} [S_1 \cdot S_2 - 3(S_1 \cdot \mathbf{n})(S_2 \cdot \mathbf{n})] - S_{1z} S_{2z} \right\} \times [I_s(z, z') + I_a(z, z')] F_2(x) \quad (26b)$$

for $x \ll v/\varepsilon_0$, where

$$I_s(z, z') = J_s(z) J_s(z') \quad I_a(z, z') = J_a(z) J_a(z')$$

$$F_1 = \frac{N_v \varepsilon_0^{1/2} \exp(-2x\varepsilon_0/v)}{4\pi^{3/2} v^{3/2} x^{5/2}} \quad F_2 = \frac{N_v}{8\pi v x^3}$$

$$F_3 = \frac{N_v \varepsilon_0^{3/2} \exp(-2x\varepsilon_0/v)}{2\pi^{3/2} v^{5/2} x^{3/2}}.$$

It should be noted that all the formulae have been derived by taking into account only one pair of nearest size-quantized levels $\varepsilon_0, -\varepsilon_0$. The contribution of remote levels should be added. For large distances, $x > v/\varepsilon_0$, owing to the factor $\exp(-2x\varepsilon_0/v)$, only the contribution of the nearest pair is relevant provided that the size quantization is not too small, i.e. $\varepsilon_1 - \varepsilon_0 \sim \varepsilon_0$.

The other restriction is related to the use of the initial Hamiltonian in the form (1). Really, this implies that levels lie deep in the QW, so that $\varepsilon_0 \ll \Delta_b$ (here $2\Delta_b$ is the energy gap in the spectrum of semiconductor outside the QW), and $k \ll \Delta_b/v$. The last condition also restricts the distances in the QW plane to $x \gg x_{\min} \sim v/\Delta_b$, for which (18) and (24) are applicable.

On the other hand, the initial Dirac model for the spectrum of a 3D semiconductor is also limited, $k \ll k_{\max} \sim E_0/v$ (where E_0 is of the order of the band width). This restriction determines the precision of calculations of envelope functions $\Phi_1(z)$ and $\Phi_2(z)$ for small z : they are applicable for $z \gg z_{\min} \sim v/E_0 \sim a_0$.

We can choose the following parameter values [9] (they correspond to PbTe/Pb_{1-x}Sn_xTe/PbTe structures with $x \leq 0.35$): $E_0 = 1$ eV, $\Delta_b = 0.2$ eV, $\varepsilon_0 = 0.02$ eV, $v = 5 \times 10^{-8}$ eV cm, $z_{\min} = 3 \times 10^{-8}$ cm, $x_{\min} = 2 \times 10^{-7}$ cm. From these estimations we see that the standard parameters of a QW on IV–VI semiconductors can satisfy the previous assumptions.

Some remarks should be made about the applicability of the initial model (1) to real IV–VI semiconductor compounds. It is known [9] that a large anisotropy of the energy spectrum can occur in some of them, so that $v_t/v_l \sim 10$ for PbTe (but remains $v_t/v_l \sim 2$ for PbSe).

Let us assume $v_t/v_l \gg 1$ and the QW to be in a (111) plane. The contribution to the magnetic density from [111] electrons (i.e. electrons in the [111] valley) is still described by (16), (18), (22) and (24) with $v = v_t$.

As for the contribution of other valleys, the whole thing is more complicated. Nevertheless, the corresponding calculations can also be performed for this case using a rescaling of both x and k [7] (and this results in the substitution $v \rightarrow (v_t v_l)^{1/2}$). On the other hand, the contribution of these valleys can be neglected because the Hamiltonian (1) for these electrons has another (much greater) value of ε_0 . Actually, for $v_t/v_l \gg 1$ we find that the corresponding quantization levels are remote compared to

the levels of the [111] valley (since the z -axis quantization is stronger for carriers which are lighter in this direction).

Thus, in the case of large anisotropy we must take $v = v_t$ and $N_v = 1$.

Another question arises about the neglecting of terms $\sim k^2$ in equation (1). They are the diagonal terms of the Dimmock model [10], and are usually written as $k^2/2m$. Since the higher-order terms become significant† for larger $k > mv$, they affect the magnetic distribution at smaller $x < 1/mv$, thus, we can neglect k^2 terms for large enough distances. Note that the condition $x \ll v/\varepsilon_0$ does not contradict the restriction $x > 1/mv$ provided that $\varepsilon_0 \ll mv^2$. We can estimate $mv^2 \sim 1$ eV [9], and the condition $\varepsilon_0 \ll mv^2$ can be fulfilled easily.

As it has been established earlier [7, 8], in bulk IV–VI crystals the indirect interaction between impurity spins depends on the distance, the angles between the spin orientations and the vector connecting the impurities. Here we have obtained the spatial distribution of spin density in the QW as well as the indirect interaction between the spins situated at arbitrary positions in the QW. In this case the interaction also depends on the spin positions inside the QW, and on the spin orientations with respect to the normal to the QW plane.

The interaction of spins in the QW can result in some ordered configurations at low temperatures. By changing the parameters of the QW and the magnetic impurity concentration we can affect the stable configurations of the impurity spins.

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† We do not consider here the special case of inverted bands.