Magnetic polarons in ferromagnetic semiconductor single-electron transistors

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Magnetic polaron (MP) formation is studied theoretically in a single-electron transistor (SET) consisting of a ferromagnetic semiconductor quantum dot (FSQD) coupled to nonmagnetic source, drain, and gate electrodes. Especially, using Green's-function technique we calculate the effect of the gate-voltage-dependent spin polarization of the charge-carrier spins on the magnetization and conductance of the ferromagnetic semiconductor SET in the Coulomb blockade regime. We apply the Anderson impurity model to the FSQD and the ferromagnetic subsystem inside the FSQD is treated in the mean-field approximation. By minimizing the total free energy of the FSQD we calculate the MP binding energy and the dot magnetization as a function of temperature and the gate voltage. The results show that the ferromagnetic transition temperature of the FSQD increases strongly due to the MP formation, which may contribute to the experimentally observed increase in the Curie temperature in the FSQD. The calculated results also indicate that due to the MP formation the average magnetization of the FSQD can be controlled by the gate voltage in a wide temperature range. Furthermore, our model predicts that the conductance vs gate-voltage curve, which in nonmagnetic SETs shows a symmetric double peak structure, becomes highly asymmetric due to the MP formation.

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I. INTRODUCTION

Nanomagnets have attracted a lot of interest both due to new basic physics found in artificial nanostructures and also due to their potential applications in spintronics and quantum information technologies.^{1,2} Especially, adding magnetic atoms to semiconductor quantum dots (QDs) in a controlled way creates new possibilities to study the interaction between the magnetic and electronic subsystems in the magnetic nanostructures under a strong spatial confinement. Moreover, the magnetic QDs could allow for a versatile control of the number of the charge carriers, spins, and the size of dots, which could lead to improved magnetic properties as compared to their bulk counterparts.³

The most studied magnetic semiconductor QD system is the (II, Mn) VI material family, which shows interesting interplay of quantum confinement and magnetism.^{4–12} Since manganese is isoelectronic with the group of II-VI compound semiconductors, it does not act as a dopant atom and the Mn-doped material typically is paramagnetic or antiferromagnetic. However, in III-V compound semiconductors, such as GaAs, manganese acts as an acceptor increasing the number of charge carriers leading, e.g., to carrier induced ferromagnetism both in thin films^{13–15} as well as in Mndoped QDs.¹⁶

The magnetic properties of the magnetic QDs are enhanced by the formation of magnetic polarons (MPs), where a charge-carrier spin trapped by an attractive potential can align spins of the magnetic atoms, thereby lowering the total free energy of the system. In the MP formation the carrier energy decreases and the carrier becomes even more localized, i.e., its wave function shrinks. Originally the MP concept was proposed by Kasuya and Yanase¹⁷ and by Nagaev¹⁸ in order to explain anomalies in the electrical conductivity in bulk ferromagnetic semiconductors. A semiclassical theory of MPs bound to charged impurities in diluted magnetic semiconductors (DMSs) was given by Dietl

and Spalek,¹⁹ and its quantum-mechanical generalization was developed by Wolff and co-workers.²⁰ Recently the MP formation has been studied intensively in magnetic (II,Mn)VI QDs and nanocrystals both theoretically^{3,10,21-26} and experimentally.^{4,5,27-29} The MP formation in magnetic QDs differs from the MPs related to single impurities in the bulk magnetic semiconductors. First, a single QD can trap several charge carriers, the number of which can be tuned with external voltages. Second, the confining potential inside the QD differs strongly from the attractive Coulomb potential of the charged impurities. An interesting new possibility in the magnetic QDs is an electrical control of the magnetic properties of the QDs.^{4,10,12}

In this paper we consider the MP formation in ferromagnetic semiconductor single-electron transistors (SETs). To make the basic physics clear we take as a starting point a simple model for the QDs in the Coulomb blockade (CB) regime based on Anderson's impurity model.³⁰ Then we add the ferromagnetic subsystem and the exchange interaction between the charge-carrier spin and the spins of the magnetic atoms to the model. We show that due to the MP formation and its dependence on the spin polarization of the charge carriers the magnetic and electrical properties of a ferromagnetic semiconductor SET can be controlled simultaneously by the gate voltage.

Our present treatment of the MP formation in QDs differs from the previous theoretical works^{3,10,21–26} in many respects: (1) in the previous treatments it has been assumed that the QDs are made of Mn-doped II-VI compound semiconductors, which are paramagnetic or antiferromagnetic without the MP effects, whereas we assume that the QD in the central region of the SET is ferromagnetic already without the MP formation. This is the case in, e.g., Mn-doped InAs QDs on a GaAs substrate.¹⁶ In ferromagnetic semiconductors the consequences of the MP formation are more prominent than in antiferromagnetic or paramagnetic materials. (2) We explicitly take into account the Coulomb repulsion between two charge carriers inside the dot, when we treat the MP formation using Anderson's impurity model in the CB regime. (3) We calculate the gate-voltage dependence of the average magnetization, the ferromagnetic ordering temperature, and the conductance in a ferromagnetic semiconductor SET, which—to the best of our knowledge—have not been considered previously. We have recently discussed³¹ the temperature and magnetic field dependences of the level broadening in magnetic semiconductor QDs and its effect on the conductance but there we neglected the MP formation.

Our work is motivated by the recent experimental results^{16,32–34} on ferromagnetic semiconductor QDs having high Curie temperatures, even above room temperature, and the first ferromagnetic semiconductor SET fabricated of Mn-doped GaAs.³⁵ Furthermore, the fabrication of electrical contacts to a single semiconductor QD has been demonstrated.³⁶ All these results indicate that ferromagnetic semiconductor SETs based on ferromagnetic QDs with high Curie temperatures are technologically feasible.

The paper is organized as follows. In Sec. II we describe the Hamiltonian applicable to a ferromagnetic semiconductor SET, which is an extension of the famous Anderson Hamiltonian to a ferromagnetic QD. In Sec. II B we calculate the retarded Green's function for the ferromagnetic semiconductor quantum dot (FSQD) in the SET. The binding energy of the MP is calculated by minimizing the total free energy of the system using the decay parameter of the dot wave function as a variational parameter. In Sec. III we present numerical results for the MP binding energy, dot magnetization, and conductance as a function of temperature and gate voltage. Finally, in Sec. IV we give some final remarks.

II. THEORY

A. Hamiltonian for the ferromagnetic SET

We assume that the SET consists of a ferromagnetic semiconductor quantum dot as a central region of the transistor coupled electrically to nonmagnetic electrodes. In our simple model for the MP formation we consider only the contribution of those charge carriers (electrons or holes) that take part in electrical conduction in the CB regime. This means that we take into account only the two uppermost singly occupied levels with energies ε_d^0 and $\varepsilon_d^0 + U$ in the dot, where U is a Coulomb repulsion parameter between two charge carriers. The lower energy levels below ε_d^0 are assumed to be irrelevant for the charge transport and the MP formation. However, they may contribute to the initial ferromagnetic ordering temperature of the background FSQD before the MP formation, as discussed below in Sec. III A. Then the Hamiltonian of the ferromagnetic SET is given by

$$H = H_A + H_m + H_{exch},\tag{1}$$

where H_A is the famous Anderson Hamiltonian,³⁰ which is given by

$$H_{A} = \sum_{\vec{k} \in S,D} E_{\vec{k}\sigma} c_{\vec{k}\sigma}^{\dagger} c_{\vec{k}\sigma} + \sum_{\sigma} \varepsilon_{d\sigma}^{0} d_{\sigma}^{\dagger} d_{\sigma} + U n_{\uparrow} n_{\downarrow}$$

$$\sigma$$

$$+ \sum_{\vec{k} \in S,D} [V_{\vec{k}\sigma} c_{\vec{k}\sigma}^{\dagger} d_{\sigma} + \text{H.c.}]. \qquad (2)$$

Here $c_{\vec{k}\sigma}^{\top}(c_{\vec{k}\sigma})$ creates (destroys) a spin- σ charge carrier with momentum $\hbar \vec{k}$ and energy $E_{\vec{k}\sigma}$ in the source (S) and drain (D) regions. The operator $d_{\sigma}^{\dagger}(d_{\sigma})$ creates (destroys) a charge carrier with spin σ on the dot and $n_{\sigma}=d_{\sigma}^{\dagger}d_{\sigma}$ with $\sigma=\uparrow$ or σ $=\downarrow$ is the occupation number operator. The last term in Hamiltonian (2) is the hybridization of the QD to the source and drain electrodes via tunneling, which gives rise to a lead coupling $\Gamma_{\sigma}=\Gamma_{\sigma}^{S}+\Gamma_{\sigma}^{D}$ with

$$\Gamma_{\sigma}^{S(D)} = 2\pi \sum_{\vec{k} \in S(D)} |V_{\vec{k}\sigma}|^2 \delta(E - E_{\vec{k}\sigma}).$$
(3)

The two last operators H_m and H_{exch} in Hamiltonian (1) distinguish it from the ordinary Hamiltonian for the nonmagnetic SETs. The magnetic subsystem, i.e., the magnetic atoms in the FSQD and their mutual ferromagnetic coupling, is described by the Heisenberg-type Hamiltonian given by

$$H_m = -\sum_{\vec{R},\vec{R}'} I(\vec{R},\vec{R}') \vec{S}_{\vec{R}} \cdot \vec{S}_{\vec{R}'} - g_L \mu_B B \sum_{\vec{R}} S_{\vec{R}}^z, \qquad (4)$$

where $I(\vec{R}, \vec{R}')$ is the ferromagnetic coupling constant between the magnetic atoms and $\vec{S}_{\vec{R}}$ is the spin operator for the total spin of the magnetic atom at a lattice site \vec{R} . The last term in Eq. (4) gives the ordinary Zeeman energy when an external magnetic field \vec{B} is in the *z* direction, i.e., in the growth direction of the dot. Using Hamiltonian (4) the average spin polarization of the magnetic atoms can be calculated in the mean-field approximation (see below).

In a ferromagnetic semiconductor SET the magnetic and electronic subsystems in the FSQD are coupled by the strong exchange interaction $H_{exch}=H_{exch}^0+V_{exch}$, which can be divided into a mean-field (static) part H_{exch}^0 and a fluctuating part V_{exch} ,

$$H_{exch}^{0} = -\frac{\Delta_{exch}}{2} (d_{\uparrow}^{\dagger} d_{\uparrow} - d_{\downarrow}^{\dagger} d_{\downarrow}), \qquad (5)$$

$$V_{exch} = -\frac{J_{exch}\Omega}{2} \sum_{\vec{R} \in \text{FSQD}} \psi_0^*(\vec{R}) \psi_0(\vec{R}) [S_{\vec{R}}^+ d_{\downarrow}^\dagger d_{\uparrow} + S_{\vec{R}}^- d_{\uparrow}^\dagger d_{\downarrow} + (S_{\vec{R}}^z - \langle S_{\vec{R}}^z \rangle) (d_{\uparrow}^\dagger d_{\uparrow} - d_{\downarrow}^\dagger d_{\downarrow})].$$

$$(6)$$

Here J_{exch} is the exchange interaction parameter, Ω is the volume of the unit cell, $\psi_0(\vec{r})$ is the wave function of the charge carrier at the dot level ε_d^0 , and Δ_{exch} is the temperature and magnetic field dependent spin-splitting parameter for the dot energy levels, and it is given by

$$\Delta_{exch}(T,B) = x\Omega J_{exch} \sum_{\vec{R} \in \text{FSQD}} |\psi_0|^2 \langle S_{\vec{R}}^z(T,B) \rangle.$$
(7)

Here *x* is the mole fraction of the magnetic atoms inside the FSQD. Typically, in the cases where the average spin polarization $\langle S_{\vec{R}}^z \rangle$ in ferromagnetic semiconductors is nonzero, the giant Zeeman splitting of the electronic states described by Eq. (7) is much larger than the ordinary Zeeman splitting given by the last term of Hamiltonian (4).

B. Retarded Green's function for the FSQD

In the calculation of the MP binding energy we assume that the charge carrier at the dot energy level ε_d^0 can be described by the ground-state wave function for a cylindrical QD (Ref. 37) having a height z_0 in the *z* direction and the radius R_0 ,

$$\psi_0(\rho, z) = \left(\frac{\sqrt{2}}{l_\omega \sqrt{\pi z_0}}\right) \sin\left[\frac{\pi}{z_0}\left(z + \frac{z_0}{2}\right)\right] e^{-\rho^2/2l_\omega^2},\qquad(8)$$

where $\rho = (x, y)$ and l_{ω} is the decay parameter, which we shall use as a variational parameter when seeking the minimum of the total energy. With the wave function [Eq. (8)] and assuming a single band with an isotropic effective mass m^* we get the following expression for the unperturbed dot energy level:

$$\varepsilon_{d}^{0} = \langle \psi_{0} | - \frac{\hbar^{2}}{2m^{*}} \nabla^{2} + V_{\text{QD}}(\rho, z) | \psi_{0} \rangle$$
$$= \frac{\hbar^{2}}{2m^{*} l_{\omega}^{2}} + \frac{\hbar^{2}}{2m^{*} z_{0}^{2}} + \frac{1}{2} m^{*} \omega^{2} l_{\omega}^{2}. \tag{9}$$

Here $V_{\text{QD}}(\rho, z)$ is the confining potential of the QD, $\omega^2 = \omega_0^2 + \omega_c^2/4$ with ω_0 as a confining parameter of the QD, and $\omega_c = eB/m^*$.

The first-order correction to the noninteracting energy level [Eq. (9)] due to the exchange interaction [Eq. (5)] is given by

$$\varepsilon_{d\sigma}^{(1)} = \varepsilon_d^0 - \frac{\Delta_{exch}}{2} (\delta_{\sigma\uparrow} - \delta_{\sigma\downarrow}). \tag{10}$$

Now, the retarded Green's function for the central region of the ferromagnetic semiconductor SET in the case of Hamiltonian (1) can be derived in the same way as in our previous paper,³¹ where we discussed the level broadening in magnetic QDs. Using Eq. (10) the final result is given by

.

$$\begin{aligned} G_{\sigma}(E) &= \langle \langle d_{\sigma}; d_{\sigma}^{'} \rangle \rangle \\ &= \frac{1 - \langle n_{\overline{\sigma}} \rangle}{E - \varepsilon_{d\sigma}^{(1)} - \Sigma_{\sigma}(E)} + \frac{\langle n_{\overline{\sigma}} \rangle}{E - \varepsilon_{d\sigma}^{(1)} - U - \Sigma_{\sigma}(E)}, \end{aligned}$$
(11)

where $\bar{\sigma}$ denotes the opposite spin to σ . The average occupation number can be calculated using Green's function (11) and the fluctuation dissipation theory,³⁸

$$\langle n_{\sigma} \rangle = -\frac{1}{\pi} \int d\omega n_F(\omega) \text{Im } G_{\sigma}(\omega + i\varepsilon).$$
 (12)

Here $n_F(\omega)$ is the Fermi-Dirac distribution function. In the case of the ferromagnetic semiconductor SET the self-energy $\Sigma_{\sigma}(E) = \Sigma_T^{\sigma}(E) + \Sigma_{exch}^{\sigma}(E)$ appearing in the Green's function (11) includes a tunneling contribution given by

$$\Sigma_T^{\sigma}(E) = \sum_{\vec{k} \in S, D} |V_{\vec{k}\sigma}|^2 / (E - E_{\vec{k}\sigma})$$
(13)

and a contribution from the exchange interaction [Eq. (6)], which can be derived following our previous treatment of the magnetic quantum wells:³⁹

$$\Sigma_{exch}^{\sigma}(E) = \left(\frac{J_{exch}\Omega}{2}\right)^{2} \sum_{\vec{R},\vec{R}'} |\psi_{0}(\vec{R})|^{2} |\psi_{0}(\vec{R}')|^{2} \left[\frac{\langle S_{\vec{R}}^{+} S_{\vec{R}'}^{-} \rangle \delta_{\sigma\downarrow}}{E - \varepsilon_{d\uparrow}^{(1)} - \Sigma_{T}^{\sigma}(E)} + \frac{\langle S_{\vec{R}}^{-} S_{\vec{R}'}^{+} \rangle \delta_{\sigma\uparrow}}{E - \varepsilon_{d\downarrow}^{(1)} - \Sigma_{T}^{\sigma}(E)} + \frac{\langle (\vec{S}_{\vec{R}} - \langle \vec{S}_{\vec{R}} \rangle) \cdot (\vec{S}_{\vec{R}'} - \langle \vec{S}_{\vec{R}'} \rangle) \rangle}{E - \varepsilon_{d\sigma}^{(1)} - \Sigma_{T}^{\sigma}(E)}\right].$$
(14)

Here $S_{\vec{R}}^{\pm} = S_{\vec{R}}^{x} \pm i S_{\vec{R}}^{y}$, and the thermal averages $\langle S_{\vec{R}}^{\alpha} S_{\vec{R}'}^{\beta} \rangle$ with $\alpha, \beta = x, y, z$ are the spin-correlation functions of the ferromagnetic lattice.

Finally, a connection of Green's function (11) to experiments is obtained by calculating the dc conductance g (Ref. 38) given by

$$g = \left(\frac{2e^2}{h}\right) \left(\frac{\Gamma_S \Gamma_D}{\Gamma_S + \Gamma_D}\right) \sum_{\sigma} \int d\omega \operatorname{Im} G_{\sigma}(\omega) \frac{\partial n_F}{\partial \omega}, \quad (15)$$

which can be determined as soon as Eqs. (11) and (12) have been solved self-consistently.

C. Magnetization of the FSQD

Due to the exchange interaction [Eq. (5)] the chargecarrier spin aligns the magnetic moments of the FSQD. In order to describe this effect we have to determine the effective molecular field created by the charge-carrier spin. It is obtainable from the poles of the magnetic Green's function $\langle \langle S_{\vec{R}}^{+}, S_{\vec{R}'}^{-} \rangle \rangle$, which can be determined from the following equation of motion (EOM):⁴⁰

$$\hbar\omega_{S}\langle\langle S_{\vec{R}}^{+}; S_{\vec{R}'}^{-}\rangle\rangle = \langle [S_{\vec{R}}^{+}, S_{\vec{R}}^{-}]\rangle + \langle\langle [S_{\vec{R}}^{+}, H]; S_{\vec{R}'}\rangle\rangle.$$
(16)

Using Hamiltonian (1) and the ordinary commutation rules for the spin operators we get

$$\begin{split} \hbar \,\omega_{S} \langle\langle S_{\vec{R}}^{+}; S_{\vec{R}'}^{-} \rangle\rangle &= 2 \langle S_{\vec{R}}^{z} \rangle \delta_{\vec{R},\vec{R}'} + \frac{J_{exch}\Omega}{2} \sum_{\sigma} |\psi_{0}(\vec{R})|^{2} \langle d_{\sigma}^{\dagger} d_{\sigma} \rangle (\delta_{\sigma\uparrow} \\ &- \delta_{\downarrow} \rangle \langle\langle S_{\vec{R}}^{+}; S_{\vec{R}'}^{-} \rangle\rangle + g_{L} \mu_{B} B \langle\langle S_{\vec{R}}^{+}; S_{\vec{R}'}^{-} \rangle\rangle \\ &+ 2 \sum_{\vec{R}''} I(\vec{R},\vec{R}'') \langle S_{\vec{R}''}^{z} \rangle \langle\langle S_{\vec{R}}^{+}; S_{\vec{R}'}^{-} \rangle\rangle \end{split}$$

+ higher order Green's functions. (17)

In this EOM there appears also higher order Green's functions, such as $\langle\langle d^{\dagger}_{\uparrow}d_{\downarrow}; S^{-}_{\vec{R'}}\rangle\rangle$, which would lead, e.g., to a second-order Ruderman-Kittel-Kasuya-Yanase (RKKY)-type effective interaction^{41,42} between the magnetic moments. This could increase further the effective molecular field acting on the magnetic moments. Here we make the same approximation as in the previous theoretical treatments^{21,22} of the MP formation and consider only the molecular field that is of the first order with respect to the exchange parameter J_{exch} . However, one must keep in mind that this approximation gives only the lower limit for the effective molecular field and therefore in reality the effect of MP formation on the magnetic properties of the QDs may be even stronger than predicted by the present first-order model.

From Eq. (17) the Green' function $\langle \langle S_{\vec{R}}^+; S_{\vec{R}'}^- \rangle \rangle$ can be solved and we obtain

$$\langle\langle S_{\vec{R}}^{+}; S_{\vec{R}'}^{-}\rangle\rangle = \frac{2\langle S_{\vec{R}}^{<}\rangle\delta_{\vec{R},\vec{R}'}}{\hbar\omega_{S} - g_{L}\mu_{B}B_{eff}(\vec{R})},$$
(18)

where the effective magnetic field acting on a magnetic atom at a position \vec{R} is given by

$$g_L \mu_B B_{eff}(\vec{R}) = g_L \mu_B B + 2 \sum_{\vec{R}'} I(\vec{R}, \vec{R}') \langle S_{\vec{R}'}^z \rangle + \frac{J_{exch}\Omega}{2} (\langle n_{\uparrow} \rangle - \langle n_{\downarrow} \rangle) |\psi_0(\vec{R})|^2, \qquad (19)$$

where the first two terms give the ordinary molecular field due to the external magnetic field *B* and the ferromagnetic spin-spin interaction between the magnetic moment and its neighboring moments. The third term in Eq. (19) describes the effect of the charge-carrier spin on the magnetic moments and it is the most important term considering the MP formation. An interesting fact is that in a ferromagnetic semiconductor SET the net spin polarization $\langle n_{\uparrow} \rangle - \langle n_{\downarrow} \rangle$ of the charge carriers inside the FSQD can be controlled by the gate voltage.³¹

In the present work we consider only the FSQDs having rather large radii ($R_0 \ge 10$ nm). Then the total number of the magnetic atoms for the mole fractions $x \ge 0.03$ is at least 100. Therefore, when we calculate the average position dependent magnetization $\langle S_{\vec{R}}^z \rangle$ of the magnetic atoms inside the FSQD caused by the effective magnetic field [Eq. (19)], we employ the local mean-field theory (LMFT). Also we consider a large dot limit, i.e., we neglect the effect of spin fluctuations beyond the LMFT on the MP formation at high temperatures. Following the previous LMFT models^{21,22} for the MP formation in QDs we assume that the average spin polarization of the magnetic atoms is a continuous function of position and it can be expressed as

$$\langle S_{\vec{R}}^{z} \rangle = SB_{S}(g_{L}\mu_{B}B_{eff}(\vec{R})/k_{B}T), \qquad (20)$$

where B_S is the Brillouin function for a magnetic atom with the total spin quantum number *S*. The average spin polarization of the FSQD is then calculated as

$$\langle S^{z} \rangle = \sum_{\vec{R} \in \text{FSQD}} \langle S_{\vec{R}}^{z} \rangle / N, \qquad (21)$$

where N is the number of unit cells inside the FSQD.

D. Total free energy of the FSQD

The MP binging energy in the ferromagnetic semiconductor SET is determined by minimizing the total free energy of the FSQD including both the electronic and ferromagnetic subsystems coupled by the exchange interaction. Using the results above we can write the total free energy as

$$F_{tot} = F_c + F_m, \tag{22}$$

where the contribution F_c from the charge carriers can be calculated using Green's function (11),

$$F_c = -\sum_{\sigma} \int \frac{dE}{2\pi} n_F(E) [2 \operatorname{Im} G_{\sigma}(E)] E.$$
 (23)

In the LMFT the magnetic contribution F_m reads

$$F_m = -k_B T \ln Z = -xk_B T \sum_{\vec{R} \in \text{FSQD}} \ln \left\{ \frac{\sinh \left[X_{\vec{R}} \left(\frac{2S+1}{2S} \right) \right]}{\sinh \left(\frac{X_{\vec{R}}}{2S} \right)} \right\},$$
(24)

where Z is the partition function of the ferromagnetic subsystem, and $X_{\vec{R}}$ is calculated using the effective molecular field [Eq. (19)],

$$X_{\vec{R}} = \frac{g_L \mu_B SB_{eff}(\vec{R})}{k_B T}.$$
(25)

The MP binding energy is defined as the energy difference

$$\Delta F_{tot} = F_{tot}(\langle S_{\vec{R}}^{z} \rangle) - F_{tot}(\langle S^{z} \rangle), \qquad (26)$$

where $F_{tot}(\langle S_{\vec{R}}^z \rangle)$ is calculated in the case of the inhomogeneous position-dependent spin polarization $\langle S_{\vec{R}}^z \rangle$ induced by the effective molecular field [Eq. (19)] and $F_{tot}(\langle S^z \rangle)$ is calculated in the case of the homogeneous spin polarization $\langle S^z \rangle$ obtained by setting $|\psi_0|=0$ in Eq. (19), i.e., by neglecting the effect of the charge-carrier spin on the average spin polarization of the FSQD. This allows us to calculate the total free energy as a function of the wave-function decay parameter l_{ω} , which is used as a variational parameter. For a given temperature and a gate voltage the total-energy difference [Eq. (26)] is minimized by varying the parameter l_{ω} . The MP is stable, if $\Delta F_{tot} < 0$. When the minimum has been found, the MP binding energy, the position-dependent spin polarization of the magnetic atoms inside the FSOD, the ferromagnetic ordering temperature, and the conductance can be determined.

III. NUMERICAL RESULTS AND DISCUSSION

A. Parameters

As a numerical example we apply our model to a disklike FSQD with a radius $R_0=10$ nm and a height $z_0=10$ nm.

Then the charging energy U can be estimated to be a few tens of millielectron volt, as calculated from the matrix element $\langle \psi_0 | e^2/4\pi\epsilon_s r | \psi_0 \rangle$ for the Coulomb repulsion between two electrons. In the numerical calculations we used the value U=20 meV. The mole fraction of magnetic atoms in the FSQD was x=0.03, which in the case of Mn-doped GaAs thin films⁴³ leads to rather low Curie temperatures, $T_{\rm C}=30-50$ K. Since we consider the MP formation only due to the charge carriers at the two highest occupied dot levels, the contribution from possible other carriers at lower energy levels is assumed to be included in the original ferromagnetic ordering before the MP formation. Therefore, the chosen Curie temperature $T_{\rm C}=2S(S+1)\Sigma_{\vec{R}}I(0,\vec{R})/3k_B=30$ K is the background ferromagnetic ordering temperature of the FSQD without the contribution from the MP formation.

The real part of the self-energy \sum_{exch}^{σ} in Eq. (14) shows a rather weak temperature dependence as compared to the first-order correction [Eq. (7)]. Therefore, we assume that $\operatorname{Re}\{\Sigma_{exch}^{\sigma}\}\$ is constant and it is included in the confining energy $\hbar\omega_0=6$ meV with $l_{\omega}=5$ nm. The Fermi energy E_F is assumed to be equal to the bottom of the confining energy of the dot, when the gate voltage is zero. The imaginary part of the self-energy [Eq. (14)] results in a spin disorder scattering³¹ of the charge carriers and the scattering rate, which is proportional to $\text{Im}\{\Sigma_{exch}^{\sigma}\}\)$, has a maximum at T $=T_{\rm C}$. However, in the calculation of the total energy the integral [Eq. (23)] does not depend strongly on the level broadening $\Gamma_{tot} = \Gamma/2 + \text{Im}\{\Sigma_{exch}^{\sigma}\}$. Therefore, in the numerical calculations we have chosen a rather large but temperatureindependent level broadening parameter Γ_{tot} =4 meV in order to see clearly the influence of the MP formation on the temperature dependence of magnetization and conductance.

The other material parameters used in the calculations were those typically found in, e.g., Mn-doped GaAs:⁴³ $m^*=0.5m_0$ (heavy holes), $J_{exch}=0.8-1.2$ eV, $a_0=5.65$ Å, and S=5/2. In the present paper all calculations have been performed in the case where the magnetic field is zero, B=0 T.

B. MP binding energy

The MP formation in the FSQD includes a shrinking of the charge-carrier wave function [Eq. (8)], i.e., a decrease in the decay parameter l_{ω} and an increase in the local spin polarization of the ferromagnetic lattice. This results in a decrease in the total free energy of the FSQD. Figure 1 shows the total-energy difference [Eq. (26)], the unperturbed dot energy [Eq. (9)], and the energy level with the first-order correction, Eq. (10) with $\sigma = \uparrow$, vs the variational parameter l_{ω} at T=20 K and at the gate voltage $V_g=10$ mV. Here the value of the gate voltage was chosen so that the level $\varepsilon_{d\uparrow}^{(1)}$ is occupied with $\langle n_{\uparrow} \rangle \approx 1$ and the level $\varepsilon_{d\downarrow}^{(1)} + U$ is empty with $\langle n_{\downarrow} \rangle \approx 0$, which maximizes the molecular field [Eq. (19)]. The minimum in the total energy is found when the wavefunction decay parameter shrinks from the original value $l_{\omega}^{0}=5$ nm to the value $l_{\omega}=1.75$ nm. The shrinking, in turn, increases the effective molecular field [Eq. (19)] and the spin polarization in the FSQD, which decreases the total free energy.



FIG. 1. Total-energy difference ΔF_{tot} (the solid curve) vs variational parameter l_{ω} in a ferromagnetic semiconductor SET at T=20 K and at a gate voltage $V_g=10$ mV in the case $J_{exch}=0.8$ eV. The dot energies ε_d^0 (the dashed-dotted curve) and $\varepsilon_{d\uparrow}^{(1)}$ (the dashed curve) as calculated from Eqs. (9) and (10), respectively, are also shown as a function of l_{ω} .

On the other hand, with the decreasing l_{ω} the kinetic energy of the charge carriers, which according to Eq. (9) is proportional to $1/l_{\omega}^2$, increases strongly, which finally leads to a strong increase in the total free energy at smaller values of the variational parameter, i.e., when $l_{\omega} < 1.7$ nm, as shown in Fig. 1.

Figure 2 shows the average occupation probabilities $\langle n_{\uparrow} \rangle$ and $\langle n_{\downarrow} \rangle$ vs l_{ω} for the dot levels $\varepsilon_{d\uparrow}^{(1)}$ and $\varepsilon_{d\downarrow}^{(1)} + U$, respectively, at a gate voltage $V_g = 10$ mV at various temperatures. Comparing Fig. 2(a) with Fig. 1 we see that at T=20 K the minimum in the total energy occurs at the value $l_{\omega}=1.75$ nm, when the net spin polarization of the charge carries reaches its maximum, $\langle n_{\uparrow} \rangle - \langle n_{\downarrow} \rangle \approx 0.9$. It is also shown in Fig. 2 that the range of the decay parameter values, for which the net



FIG. 2. Average occupation probabilities $\langle n_{\uparrow} \rangle$ and $\langle n_{\downarrow} \rangle$ vs l_{ω} for the dot levels $\varepsilon_{d\uparrow}^{(1)}$ and $\varepsilon_{d\downarrow}^{(1)} + U$, respectively, at a gate voltage $V_g = 10$ mV at various temperatures in the case $J_{exch} = 0.8$ eV. The arrows refer to the direction of the charge-carrier spin σ .



FIG. 3. MP binding energy vs temperature for various gate voltages in a ferromagnetic semiconductor SET in the case J_{exch} =0.8 eV. The integers refer to the gate voltages as follows: 1=-10 mV, 2=10 mV, 3=50 mV, 4=100 mV, 5=200 mV, and 6=400 mV.

spin polarization $\langle n_{\uparrow} \rangle - \langle n_{\downarrow} \rangle$ is nonvanishing, becomes narrower with increasing temperature.

Figure 3 shows the MP binding energy vs temperature in a ferromagnetic semiconductor SET for various gate voltages. An interesting property is the strong dependence of the binding energy on the gate voltage: both the value of the binding energy and the temperature range, where the MP formation occurs, can be controlled by the gate voltage. This is due to the fact that in a ferromagnetic semiconductor SET the net spin polarization of the charge carriers, to which the effective molecular field [Eq. (19)] is proportional, depends on the gate voltage. At negative and small positive voltages the Fermi level is below the dot energy level $\varepsilon_{d\uparrow}^{(1)}$ and the occupation probability of the level is small. This means a small effective molecular field [Eq. (19)] and the MP is stable only in a narrow temperature range at gate voltages $V_{o} < 10$ mV, as shown in Fig. 3. Also the minimum of the total free energy is reached at rather large values of the decay parameter, $l_{\omega} \approx 3$ nm. At higher gate voltages there are smaller values of the parameter l_{ω} , for which the energy level $\varepsilon_{d\downarrow}^{(1)}$ with $\langle n_{\uparrow} \rangle \approx 0.9$ is still below the Fermi level but the level $\varepsilon_{d\downarrow}^{(1)} + U$ is unoccupied with $\langle n_{\downarrow} \rangle \approx 0$. The large shrinking of the wave function leads to a strong increase in the molecular field [Eq. (19)] at the center of the dot since the field is proportional to $1/l_{\omega}^3$. Therefore, at higher gate voltages the MP is stable at higher temperatures as shown in Fig. 3. It is interesting to note that both the Coulomb blockade with a large value for U and the giant Zeeman splitting [Eq. (7)] favor the MP formation by increasing the separation between the spin-up and spin-down dot energy levels, and thereby increasing the net spin polarization $\langle n_{\uparrow} \rangle - \langle n_{\downarrow} \rangle$ and the molecular field [Eq. (19)].

Figure 4 shows the shrinking of the MP wave function as a function of the gate voltage at T=20 K. One should note



FIG. 4. Decay parameter of the MP wave function vs gate voltage in a ferromagnetic semiconductor SET at T=20 K in the case $J_{exch}=0.8$ eV.

that the strong dependence of the wave function on the rather small changes in the gate voltage is a unique feature of the ferromagnetic semiconductor SET.

C. Spin polarization of the FSQD

The position-dependent nonuniform spin polarization of the ferromagnetic lattice inside the FSDQ is shown in Fig. 5. At low temperatures well below the original Curie temperature $T_C=30$ K the whole QD is spin polarized and the position dependence of the spin polarization is weak. At temperatures $T \ge T_C$ the exponential decay of the MP wave function $\psi_0(R)$ and the consequent large position dependence of the effective molecular field [Eq. (19)] lead to a strong decrease in the spin polarization with the increasing position argument R. At higher temperatures only the center of the FSQD is spin polarized until the whole MP disappears. This results in a small remnant spin polarization of the FSQD at temperatures much higher than the original Curie temperature, as



FIG. 5. Spin polarization of the ferromagnetic lattice vs position inside the FSQD in a SET at various temperatures at a gate voltage $V_g=50$ mV in the case $J_{exch}=0.8$ eV and $T_C=30$ K.



FIG. 6. Temperature dependence of the average spin polarization of the FSQD as calculated from Eq. (21) for various values of the gate voltage in the case $J_{exch}=0.8$ eV. The integers refer to the following values of the gate voltage: 1=-10 mV, 2=50 mV, 3=100 mV, 4=200 mV, and 5=400 mV. The dashed curve shows the uniform spin polarization vs temperature, when the MP formation is neglected. The dashed-dotted curve shows the spin polarization vs temperature in the case of the MP formation at V_g =400 mV, when the exchange parameter is increased from $J_{exch}=0.8$ eV to $J_{exch}=1.2$ eV.

long as the MP is stable. This is shown in Fig. 6. The temperature dependence of the average spin polarization of the FSOD, which is described by the Brillouin function if the MP effects are neglected (the dashed curve in Fig. 6), becomes weaker when the MP formation is included. Due to the MP formation there is a long tail in the spin polarization vs temperature curve and the ferromagnetic transition temperature, which is defined as the minimum temperature where the spin polarization vanishes, increases significantly. The ferromagnetic transition temperature increases up to 227 K, if the exchange interaction parameter J_{exch} is increased from 0.8 to 1.2 eV, as shown in Fig. 6. Similar weakening of the temperature dependence of the spin polarization from the one described by the Brillouin function has been predicted for the III-V DMS thin films.44 This behavior has been found experimentally already in the first reported observation¹³ of ferromagnetism in (In,Mn)As (for more experimental results see also Ref. 45 and references therein). Our model predictions indicate that the MP formation could contribute to the observed temperature dependence of the spin polarization also in the case of ferromagnetic semiconductor thin films, if there are small clusters of magnetic atoms or if the film consists of ferromagnetic nanocrystals of the size of the FSOD considered in the present work.

An interesting prediction of our MP model for ferromagnetic semiconductor SETs is the possibility to control the dot magnetization and the ferromagnetic ordering temperature through the gate voltage, as shown in Fig. 6. In a wide temperature range one can switch on and off the spin polarization of the dot by changing the gate voltage, e.g., from 0 to 100 mV, as shown in Fig. 7. Also the Curie temperature can be increased from the original value $T_{\rm C}$ =30 K to above 160 K by increasing the gate voltage from 0 to 400 mV, respectively, as shown in Fig. 8. The calculated results shown in



FIG. 7. Dependence of the spin polarization on the gate voltage at various temperatures in a ferromagnetic semiconductor SET in the case $J_{exch}=0.8$ eV.

Figs. 6 and 8 indicate that the MP formation could contribute to the experimentally observed¹⁶ increase in the Curie temperature in the FSQDs as compared to their thin-film counterparts.

D. Conductance

In the case of the MP formation we can calculate its effect on the conductance using the retarded Green's function (11)and the conductance expression (15). From the latter equation we see that since $\partial n_F / \partial E \approx \delta(E - E_F)$ at low temperatures only the electronic states near the Fermi energy E_F contribute to the electrical transport. Therefore the change in the Fermi energy E_F due to the change in the gate voltage scans the density of states (DOS), or $-2 \text{ Im } G_{\sigma}$, and the two peaks in the DOS at the energies $\varepsilon_{d\uparrow}^{(1)}$ and $\varepsilon_{d\downarrow}^{(1)} + U$ appear also in the conductance vs gate-voltage curves. This is shown in Fig. 9, where the gate-voltage dependence of the conductance in a ferromagnetic SET is depicted at various temperatures both in the presence and absence of the MP formation. In the former case two symmetric CB peaks, separated by a voltage U/e, are shown. The ordinary thermal wash out of the peaks appears with increasing temperature. However, in the case of the MP formation the symmetry in the doublepeak structure is broken. Especially the second peak at the energy level $\varepsilon_{d}^{(1)} + U$ almost disappears or it is shifted to higher gate voltages with the increasing temperature, when



FIG. 8. Dependence of the ferromagnetic ordering temperature on the gate voltage in a ferromagnetic semiconductor SET in the case $J_{exch}=0.8$ eV.



FIG. 9. Conductance, in units of $(e^2\Gamma_{tot}/\hbar U)$, vs gate voltage at various temperatures in a ferromagnetic semiconductor SET in the case $J_{exch}=0.8$ eV. The solid curves have been calculated without the MP effects, whereas in the case of the dashed curves the MP formation is included. Notice a different gate-voltage scale in (d), as compare to (a)–(c).

the MP is formed. This is due to the fact that when the MP is formed at gate voltages $eV_g \ge \varepsilon_{d\downarrow}^{(1)}$, the orbit of the MP wave function shrinks and the kinetic energy increases, which then shifts the level $\varepsilon_{d\downarrow}^{(1)} + U$ above the Fermi level, or the Fermi level matches the level $\varepsilon_{d\downarrow}^{(1)} + U$ at higher gate voltages. It is interesting to note in Fig. 9(d) that at T=90 K, where the double-peak structure already vanishes in the absence of MP formation, it appears again in the case of the MP formation. However, now the energy separation between the first and second peaks is not due to the CB effect but due to the MP formation at high gate voltages. From the experimental point of view the asymmetry of the conductance shown in Fig. 9 is a signature, which clearly distinguishes the electrical behavior of the ferromagnetic semiconductor SET from the one typically observed in nonmagnetic SETs.

IV. CONCLUSIONS

We have analyzed theoretically the MP formation and charge transport in a ferromagnetic semiconductor SET,

where a ferromagnetic quantum dot is coupled electrically to nonmagnetic electrodes. Our model predicts that the strong exchange interaction between the charge-carrier spins and the localized spins of the magnetic atoms inside the dot causes the MP formation, which then enhances the magnetization of the dot and increases significantly the ferromagnetic ordering temperature. An interesting prediction of our model is the control of the ferromagnetic properties of the dot through the gate voltage due to the strong dependence of the MP formation on the gate voltage. Therefore, the ferromagnetic semiconductor SET may even provide a highly miniaturized memory element in the future. The most prominent difference in the electrical behavior between the ferromagnetic semiconductor SET and the ordinary nonmagnetic SET is the highly asymmetric conductance vs gate-voltage curve due to the MP formation in magnetic SETs. Especially, our model predicts that when the MP is formed at high gate voltages the original single conductance peak splits into two peaks also at high temperatures.

It is a straightforward task to improve our simple model, e.g., by taking into account the RKKY-type contribution to the effective molecular field caused by the charge-carrier spin-mediated additional coupling between the magnetic atoms in the dot. In the present model we have considered only the charge carriers at the two uppermost occupied electronic states in the dot and their role in the MP formation. However, the other charge carriers at the lower electronic states may contribute especially to the magnetic properties of the dot. Also, in order to get more reliable quantitative predictions in the case where the holes act as charge carriers, one should consider the detailed valence band structure including the heavy and light holes as well as the split-off band, when the electronic structure of the dots made of III-V DMS is calculated. However, we believe that our simple model gives the correct qualitative predictions for the MP formation in ferromagnetic semiconductor SETs and its effects on the magnetic and electrical behaviors of the transistor, such as the large increase in the ferromagnetic ordering temperature and its gate-voltage dependence.

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