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ELECTRONIC PROPERTIES OF SOLID

Spin-Flip Induction of Fano Resonance upon Electron Tunneling through Atomic-Scale Spin Structures[1]

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Abstract—The inclusion of inelastic spin-dependent electron scatterings by the potential profiles of a single magnetic impurity and a spin dimer is shown to induce resonance features due to the Fano effect in the transport characteristics of such atomic-scale spin structures. The spin-flip processes leading to a configuration interaction of the system's states play a fundamental role for the realization of Fano resonance and antiresonance. It has been established that applying an external magnetic field and a gate electric field allows the conductive properties of spin structures to be changed radically through the Fano resonance mechanism.

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1. INTRODUCTION

The possibility of probing nanosystems with the needle of a scanning tunneling microscope (STM) has made the transition to studying the charge and spin-dependent transport at the level of individual atoms and molecules real [1–8]. In particular, it has been shown in recent years that it is possible in principle to determine the spin configuration of atomic and molecular systems and to control their spin state via the inelastic action of a current due to an exchange interaction between the carrier spin moments and the localized spins of the structure [9, 10]. Such electric control allows one to count on the application of magnetic nanoobjects as logic and memory elements [8, 11] and as basic elements for quantum computing [12]. Using STM has allowed one to observe experimentally the Zeeman splitting of energy levels in an individual manganese atom [1], to confirm the antiferromagnetic nature of the exchange coupling in chains of atoms and magnetic molecules based on transition metals [2, 4, 7], and to establish a magnetic anisotropy for such systems with spin $S > 1/2$ [3, 6]. The transport properties of single magnetic molecules in tunneling contract with electrodes appear attractive from the viewpoint of future applications of molecular spintronics. Calculations for a break-junction geometry showed that a single magnetic molecule could function as a spin filter if it was bridged between paramagnetic metal electrodes [13]. In addition, this molecule operates on the principle of a spin diode if it is between ferromagnetic electrodes with different carrier spin polarizations [14].

In the case of a strong coupling, the formation of a multiparticle ground state according to the Kondo scenario is responsible for the appearance of a resonance peak in the differential conductance of a magnetic nanoobject at low temperatures [15, 16]. However, it was shown in [17] that this feature could have a significantly asymmetric shape. This is because there is interference between the system's states corresponding to two channels for electron tunneling through a magnetic impurity: the first—through the discrete state of the *d* orbital of a cobalt atom and the second—directly into the continuum states of the conduction band of a gold substrate. The described mechanism proposed by Fano [18] is possible only in the case of coherent electron transport achieved through the short lifetime of conduction electrons on the *d* orbital of cobalt [19].

Here, we analyze the appearance of Fano resonance features in the electron tunneling transport characteristics for two atomic-scale spin structures that have been actively investigated in recent years in experiments with the application of STM. The first spin system is a single impurity with single-ion anisotropy. For this system, the spin-flip processes due to the exchange interaction with the electron being transported can induce the Fano effect in a certain energy range. In this case, the transport characteristic of the magnetic impurity contains an asymmetric peak. As the second spin structure, we chose a spin dimer in which the spin moments are coupled by an antiferromagnetic interaction. Just as in the first case, the spin-flip processes play a significant role in producing the Fano effect and modifying the transport characteris-

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tics of the spin dimer. We studied the influence of the gate electric field and magnetic field on the realization of Fano resonances. We calculated the magnetoresistance of a system containing one of the spin structures under consideration as an active element by the Landauer method.

2. THE HAMILTONIAN OF A SYSTEM WITH A MAGNETIC IMPURITY

Consider the quantum transport of an electron through a region containing a magnetic impurity with spin $\mathbf{S} = 1$ in tunneling contact with one-dimensional metallic electrodes. In this case, the left and right electrodes correspond to the STM needle and the metallic substrate, respectively. The tunneling coupling to the right lead in our experiment is achieved through the adsorption of magnetic atoms on a dielectric nanolayer. This situation in the strong-coupling model (tight-binding approximation) is shown in Fig. 1.

The Hamiltonian of the system being studied under the adopted assumptions can be written as

$$\hat{H} = \hat{H}_L + \hat{H}_R + \hat{H}_{TR} + \hat{H}_{De} + \hat{H}_{ex} + \hat{H}_I, \qquad (1)$$

where $\hat{H}_L$ and $\hat{H}_R$ are the operators that allow for the presence of electronic states in the left and right semi-infinite metallic electrodes, respectively. In an experimental situation, these electrodes can be made of one metal. Therefore, the first two terms of Hamiltonian (1) are described by the expression

$$\hat{H}_\alpha = \sum_{n \in \alpha;\, \sigma} [\varepsilon_{\alpha\sigma} c^\dagger_{n\sigma} c_{n\sigma} + t(c^\dagger_{n\sigma} c_{n-1,\sigma} + c^\dagger_{n-1,\sigma} c_{n\sigma})],$$

where $c^\dagger_{n\sigma}$ ($c_{n\sigma}$) is the creation (annihilation) operator for a conduction electron with spin σ on site n of electrode α ($\alpha = L, R$); $t < 0$ is the hopping parameter between electrode sites. For simplicity, we will assume the single-electron energy ε_α on a site of electrode α to be equal to the system's Fermi energy E_F. The quantity $\varepsilon_{\alpha\sigma} = -g_e \mu_B H\sigma$ is then the Zeeman energy of an on-site electron with spin σ in an external magnetic field $\mathbf{H}$. The z axis along which the magnetic field is directed is perpendicular to the direction of electron motion.

The third term in Eq. (1) describes the conduction electron hops between the leads and the central region:

$$\hat{H}_{TR} = \sum_\sigma t_{TR}(c^\dagger_{1\sigma} c_{0\sigma} + c^\dagger_{0\sigma} c_{1\sigma} + c^\dagger_{2\sigma} c_{1\sigma} + c^\dagger_{1\sigma} c_{2\sigma}),$$

where $t_{TR} < 0$ is the tunneling hopping parameter (see Fig. 1), $|t| > |t_{TR}|$. The fourth term of the Hamiltonian describing the energy of an on-site electron with spin $\mathbf{S}$ has a simple form, $\hat{H}_{De} = \sum_\sigma \varepsilon_{D\sigma} c^\dagger_{1\sigma} c_{1\sigma}$. Here, in contrast to the banks, $\varepsilon_D \neq E_F$ and $\varepsilon_{D\sigma} = \varepsilon_D - g_e \mu_B H\sigma$. The quantity ε_D is known to reflect the influence of the

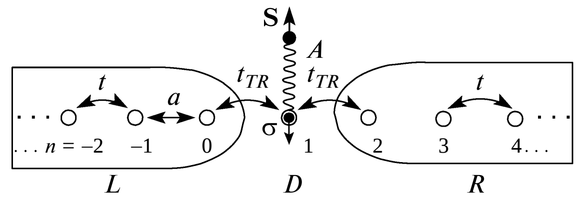

Fig. 1. Single magnetic impurity with spin **S** located between the left ($n \le 0$) and right ($n \ge 2$) metallic electrodes.

transverse gate electric field and, as will be shown below, this field can play a significant role in observing the Fano effect in the tunneling regime.

Given the above remarks, the interaction of the electron being transported with the impurity is defined by the term $\hat{H}_{ex}$:

$$\hat{H}_{ex} = \frac{A}{2}[(c^\dagger_{1\uparrow} c_{1\downarrow} S^- + c^\dagger_{1\downarrow} c_{1\uparrow} S^+) + (n_{1\uparrow} - n_{1\downarrow}) S^z], \qquad (2)$$

where A is the exchange interaction parameter; S^+, S–, and S^z are the impurity spin moment operators.

As follows from the experimental data, a distinct magnetic anisotropy is observed in individual manganese and iron atoms [3, 5]. In the simplest case, such a system in an external magnetic field is described by the Hamiltonian

$$\hat{H}_I = D(S^z)^2 - g\mu_B H S^z, \qquad (3)$$

where $D > 0$ is the anisotropy constant, g is the Lande factor of the impurity. Thus, as follows from (3), the magnetic impurity has a set of energy levels classified by its spin projection, S^z. At $D > g\mu_B H$, the singlet state ($S^z = 0$) is the impurity's ground state.

3. THE FANO EFFECT UPON TUNNELING THROUGH A SINGLE IMPURITY

Following the reasoning used in [20, 21], about the form of the solution of the Schrodinger equation when inelastic spin-dependent scatterings are present in the system, we will seek a wave function in the form

$$|\Psi_L\rangle = \sum_n [w_n c^\dagger_{n\uparrow} \chi_0 + u_n c^\dagger_{n\downarrow} \chi_1]|0\rangle. \qquad (4)$$

In writing (4), we assume an electron with a spin projection of 1/2 to be injected by the left lead when the impurity is in its ground singlet state χ_0. The spin-flip processes induce the impurity's transition to an excited state χ_1 with a spin moment projection $S^z = 0$; $|0\rangle$ is the vacuum state for the fermionic subsystem.

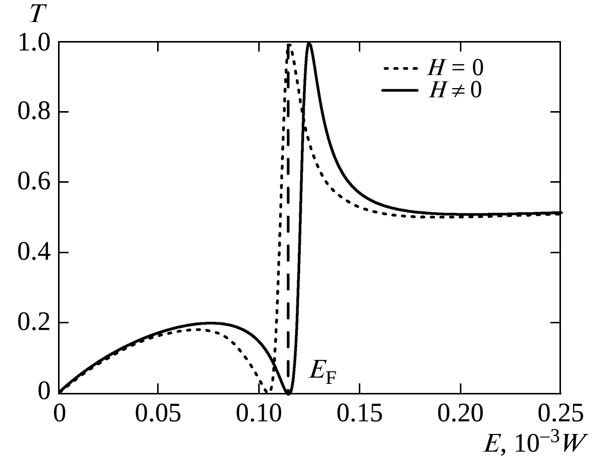

Fig. 2. Low-energy region of the dependence $T(E)$ for the tunneling coupling of a magnetic impurity to the electrodes, $t = -1$ eV, $\tau \approx 0.25$, $\varepsilon_D \approx -0.47$, $D = A = 0.25 \times 10^{-3}$, $\mu_B H = 1 \times 10^{-4}$, $g = 1$.

The expressions for the partial amplitudes can be written as

$$n \le 0:\ w_n = e^{ikn} + r_0 e^{-ikn}, \quad u_n = r_1 e^{-iqn},$$
$$n \ge 2:\ w_n = t_0 e^{ikn}; \quad u_n = t_1 e^{iqn}, \tag{5}$$

where $r_0(t_0)$ and $r_1(t_1)$ are the reflection (transmission) amplitudes when the impurity is in the ground and excited states, respectively. The wave vectors k and q satisfy the dispersion relations

$$E = (1 - \cos k)/2,$$
$$E = D + (2 - g)\mu_B H + (1 - \cos q)/2. \tag{6}$$

Here and below, all energy quantities are measured in units of the band width $W = 4|t|$. In writing Eqs. (6), we changed the electron energy by $-1/2 - \mu_B H$.

Previously [21], we showed that at energies of the electron being transported below the energy of the excited state of an impurity in a magnetic field, $D - g\mu_B H$, the electron transmission coefficient T is characterized by the Fano effect. This feature appears as an antiresonance of the transmission coefficient ($T = 0$) at $t = t_{TR}$. Such a behavior is a consequence of destructive interference between the electron waves relating to the continuum state, $c^\dagger_{n\uparrow}\chi_0|0\rangle$, and the state of a discrete spectrum, $c^\dagger_{n\downarrow}\chi_1|0\rangle$.

As a result of solving the Schrodinger equation for $t \ne t_{TR}$, we will obtain the following expression for the tunneling transmission coefficient through a magnetic impurity in the low-energy regime, $E < D + (2 - g)\mu_B H$:

$$T = |t_0|^2 = \tau^4 D_q^2 \sin^2 k / \{\tau^4 D_q^2 \sin^2 k + [[(1 - \tau^2)\cos k + 2\varepsilon_D] D_q + A^2]^2\}, \tag{7}$$

where $D_q = (\tau^2 e^{iq} - \cos q + A)/2 - \varepsilon_D$, $\tau = |t_{TR}|/|t|$. It follows from Eq. (7) that, in contrast to the situation where $t = t_{TR}$, resonant electron transmission ($T = 1$) is also possible in the tunneling regime in addition to the T antiresonance. The dotted ($H = 0$) and solid ($H \ne 0$) curves in Fig. 2 indicate the Fano peaks that have a characteristic asymmetric shape with closely spaced reflection and transmission resonances [19]. As can be seen, the action of the magnetic field on the Fano peak is reduced to its shift.

The expression for the Fano antiresonance energy is

$$E_{\text{ares}} = D + (2 - g)\mu_B H + \frac{1}{2}\{1 - [(1 - \tau^2)(A - 2\varepsilon_D) - \tau^2\sqrt{(A - 2\varepsilon_D)^2 + 2\tau^2 - 1}]/(1 - 2\tau^2)\}. \tag{8}$$

At $\tau \ll 1$ and $A \ll 1$ (in energy units, $A \sim 1$ meV [22]), the radicand in (8) is negative if $\varepsilon_D = 0$. Thus, the gate electric field allows the Fano resonance energies to be brought into the real domain in the tunneling regime and can serve as an efficient mechanism for observing the Fano resonances under experimental conditions, because $\varepsilon_D \sim 1$ eV in the experiment [23].

It is worth emphasizing that the transverse part of the operator $\hat{H}_{ex}$ responsible for the spin-flip processes plays a fundamental role for observing the Fano effect upon transport through such spin structures. In our case, taking into account precisely this component in (2) leads to the "mixing" of an excited state into the wave function (4).

4. THE FANO EFFECT UPON TRANSPORT THROUGH A SPIN DIMER

An important role of the spin-flip processes and external magnetic field in the appearance of Fano resonance features is revealed when analyzing inelastic spin-dependent electron transport through the potential profile of another spin structure. It is formed from two spin moments, $\mathbf{S}_1 = 1/2$ and $\mathbf{S}_2 = 1/2$, coupled by an exchange antiferromagnetic interaction and forming a spin dimer. The Hamiltonian of a dimer in a magnetic field can be written as

$$\hat{H}_D = J(\mathbf{S}_1 \cdot \mathbf{S}_2) - g\mu_B H(S_1^z + S_2^z), \tag{9}$$

where $J > 0$ is the intradimer exchange interaction parameter, g is the Lande factor of the dimer. Below, just as in the preceding part, we will consider the case of a weak magnetic field ($g\mu_B H < J$). Therefore, the singlet state D_{00} (the first and second indices denote the total spin and its projection, respectively) will be the dimer's ground state.

Since the tunneling matrix element for a magnetic atom located immediately under the STM needle is dominant in most cases [9], our subsequent calculations will be based on the fact that the electron being transported interacts only with the first spin moment of the dimer, $\mathbf{S}_1$. Thus, the exchange interaction Hamiltonian $\hat{H}_{ex}$ is the same in form as operator (2). However, in contrast to the previous case, the dimer can pass from the initial singlet state D_{00} to two triplet states, D_{10} and D_{11}, as a result of this interaction. This is reflected in the form of the wave function,

$$|\Psi_L\rangle = \sum_n [w_n c_{n\uparrow}^\dagger D_{00} + u_n c_{n\uparrow}^\dagger D_{10} + v_n c_{n\downarrow}^\dagger D_{11}]|0\rangle. \tag{10}$$

Here, the partial amplitudes w_n, u_n, and v_n can be written as

$$\begin{aligned} n \le 0:\ & w_{n\uparrow} = e^{ikn} + e_{00}e^{-ikn}; \\ & u_{n\uparrow} = r_{10}e^{-iqn}; \quad v_{n\downarrow} = r_{11}e^{-ipn}; \\ n \ge 2:\ & w_{n\uparrow} = t_{00}e^{ikn}; \\ & u_{n\uparrow} = t_{10}e^{iqn}; \quad v_{n\downarrow} = t_{11}e^{ipn}, \end{aligned} \tag{11}$$

where $r_{00}(t_{00})$, $r_{10}(t_{10})$, and $r_{11}(t_{11})$ are the reflection (transmission) amplitudes when the dimer is in the singlet and triplet states, respectively; k, q, and p are the wave vectors satisfying the relations

$$\begin{aligned} E = (1-\cos k)/2, \quad E = J + (1-\cos q)/2, \\ E = J + (2-g)\mu_B H + (1-\cos p)/2. \end{aligned} \tag{12}$$

In writing these relations, we changed the electron energy by $-1/2 - 3J/4 - \mu_B H$. It follows from Eqs. (12) that the probability density for the system to be in the states $c_{n\uparrow}^\dagger D_{10}|0\rangle$ and $c_{n\downarrow}^\dagger D_{11}|0\rangle$ at $E < J$ will decay exponentially, which creates prerequisites for the Fano effect.

The transmission coefficient through the spin dimer at $E < J$ is

$$\begin{aligned} T &= |t_{00}|^2 = \frac{\alpha^2}{\alpha^2+1}, \\ \alpha &= -\frac{4\tau^2[\Omega(C_2+A) + 2\Delta C_2]\sin k}{\Omega[4C_1(C_2+A) + 3A^2] + 2\Delta(4C_1C_2 + A^2)}, \end{aligned} \tag{13}$$

where

$$\begin{aligned} C_1 = (1-\tau^2)\cos k + 2\varepsilon_D, \quad \Omega = 2C_2 - A, \\ \Delta = C_3 - C_2, \\ C_2 = \tau^2 e^{iq} - \cos q - 2\varepsilon_D, \\ C_3 = \tau^2 e^{ip} - \cos p - 2\varepsilon_D. \end{aligned} \tag{14}$$

Figure 3 shows the behavior of the function $T(E)$ at low energies. Two asymmetric Fano peaks can be seen on the plot. The shift in the Fano antiresonance of the first of the peaks is shown in the lower inset of the fig-

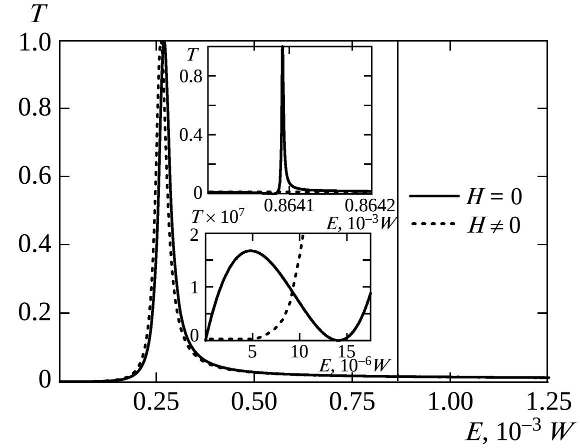

Fig. 3. Low-energy region of the dependence $T(E)$ upon transport through a spin dimer, $t = -1$ eV, $\tau = 0.075$, $J = A = 1.25 \times 10^{-3}$, $\mu_B H = 1.25 \times 10^{-4}$, $\varepsilon_D = -0.498$, $g = 1.88$. The structure of the induced asymmetric peak is shown in the upper inset. The shift of the antiresonance with energy E_{ares1} in a magnetic field is shown in the lower inset.

ure. As follows from (13), its energy at $H = 0$ can be found from the equation $C_2 + A = 0$ to be

$$\begin{aligned} E_{\text{ares1}} = J - \{2\varepsilon_D + 1 - A + \tau^2 \\ \times [\sqrt{(2\varepsilon_D - A)^2 + 2\tau^2 - 1} \\ - 2\varepsilon_D - 2 + A]\}/2(2\tau^2 - 1). \end{aligned} \tag{15}$$

It can be seen from the upper inset that one of the asymmetric Fano peaks disappears at $H = 0$. Concurrently, the quantity Ω is canceled in the transmission coefficient. Having solved the equation $\Omega = 0$, we obtain the following approximate energy of the antiresonance induced by the magnetic field:

$$\begin{aligned} E_{\text{ares2}} \approx J - \Big\{2\varepsilon_D + 1 + \frac{A}{2} \\ + \tau^2[\sqrt{(2\varepsilon_D + A/2)^2 + 2\tau^2 - 1} \\ - 2\varepsilon_D - 2 - A/2]\Big\}/2(2\tau^2 - 1). \end{aligned} \tag{16}$$

In contrast, from a physical viewpoint, switching on the magnetic field causes the triplet state energy degeneracy to be removed and, as a consequence, an additional energy scale on which the electron waves interfere emerges and a new Fano peak appears. Thus, in the case of a dimer, the action of the magnetic field is reflected not only in a shift of the Fano peak but also in the appearance of an additional peak. It follows from Eqs. (15) and (16) for the antiresonance energies that applying the gate electric field can allow the Fano resonance features to be observed with STM.

To assess the role of the spin-flip processes in forming the Fano resonances, let us analyze several special cases of transport through a dimer differing by the

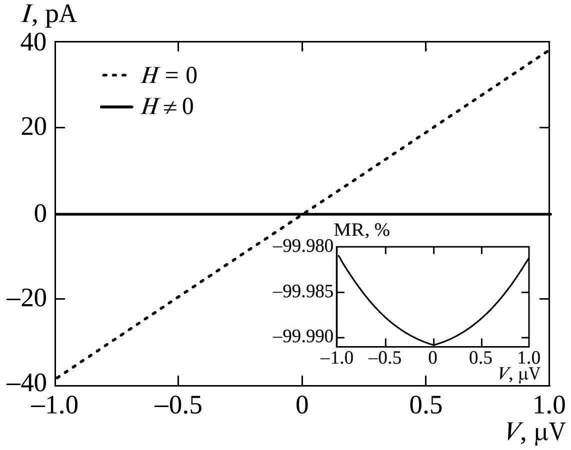

Fig. 4. Current–voltage characteristic of a system with a magnetic impurity for the parameters of Fig. 2, $E_F = 0.115 \times 10^{-3}$. The system's magnetoresistance is shown in the inset.

form of the exchange interactions in the system. If the operator $\hat{H}_{ex}$ has the Ising form and $\hat{H}_D$ remains as before, then the initial configuration $c_{n\uparrow}^{\dagger}D_{00}|0\rangle$ can pass only to the state $c_{n\downarrow}^{\dagger}D_{10}|0\rangle$. Consequently, one continuum state and one localized state are possible in the system and no new Fano resonance will be induced by the magnetic field. Let us turn to the opposite situation where $\hat{H}_{ex}$ and $\hat{H}_D$ have the Heisenberg and Ising forms, respectively. In this case, the ground state of the dimer is doubly degenerate, because two states, $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$, have the energy $E_{00} = -I/4$. However, the action of the magnetic field does not give rise to a new Fano peak in this case either, because there is only one excited state, $|\uparrow\uparrow\rangle$. If, alternatively, there are no transverse components in both exchange Hamiltonians, then the transport will be accomplished only through the system's initial state. In this case, the problem is reduced to standard particle scattering by a potential with power A. Thus, the induction of an additional Fano peak by a magnetic field upon transport through a spin dimer is possible only when the spin-flip processes in the system are completely taken into account.

5. ANOMALOUSLY HIGH MAGNETORESONANCE DUE TO THE FANO EFFECT

In conclusion, note that the demonstrated influence of a magnetic field on the Fano resonances can be responsible for the appearance of an anomalously high magnetoresistance. Figure 4 shows the current–voltage characteristics of a system with a single magnetic impurity calculated by assuming the states near the Fano peak to be current-carrying ones (see the position of the Fermi energy, E_F, denoted by the dashed straight line in Fig. 2). We calculated the current–voltage characteristic within the Landauer approach,

$$I(V) = \frac{e}{h}\int dE\,T(E)[f_L(E) - f_R(E)], \qquad (17)$$

where $f_L(E) \equiv f(E - \mu_L)$ and $f_R(E) \equiv f(E - \mu_R)$ are the Fermi electron distribution functions in the left and right leads, respectively, with electrochemical potentials $\mu_L = E_F$ and $\mu_R = E_F - eV$. The transmission coefficient was calculated by taking into account the applied external electric field eV in Hamiltonian (1). As can be seen from Fig. 4, there is virtually no current at $H \neq 0$, because the electron energy is in the Fano antiresonance region. The difference in the behavior of the differential conductance, $G(V) = dI/dV$, leads us to conclude that such a device has a magnetoresistance due to the Fano effect, $\mathrm{MR} = [G(H)/G(0) - 1] \times 100\%$. Its value in the case under consideration reaches almost 100% (see the inset in Fig. 4).

6. CONCLUSIONS

We investigated the effects of inelastic spin-dependent tunneling transport through atomic-scale spin structures: a single magnetic impurity and a spin dimer. These structures have a set of ground singlet and excited states. The exact solution of the Schrodinger equation within the strong-coupling method allowed the transmission coefficients through spin structures characterized by the presence of Fano resonance features to be calculated. We pointed out that under the assumption of a tunneling coupling between the electrodes and the spin structure, the Fano antiresonance energies become complex in the absence of a gate electric field. Allowance for the spin-flip processes in the system was shown to play a fundamental role for realizing the Fano effect in the case of a magnetic impurity and inducing the Fano peak by a magnetic field in the case of a spin dimer. We showed within the Landauer formalism that the influence of a magnetic field on the Fano resonances could be responsible for the appearance of an anomalously high magnetoresistance in a device in which the spin structures considered acted as active elements.

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