Electronic properties of atomic ribbons with spin-orbit couplings on different substrates

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I. INTRODUCTION

The electron transport properties of atomic chains have been the subject of many theoretical and experimental papers mainly due to their potential applications in nanoelectronics and quantum computing. Modern experimental techniques make it possible to fabricate one-atom thick ribbons or atomic chains, which are the thinnest possible electric wires. 1–4 Semiconductor nanochains are good candidates for application in electronic nanodevices like logic gates or field effect transistors. 5,6 Such quasi-one-dimensional systems reveal many interesting effects like conductance quantization, 7–9 conductance oscillations, 10–12 photon-assisted tunneling, 13,14 Friedel oscillations and charge density waves, 15,16 spin-charge separation, 17 and others. Chains with spin-orbit interactions coupled with the superconductor electrode can reveal nontrivial topological phases with Majorana zero modes 18–20 at both chain ends. Similarly, spinless topological states were predicted in the Su-Shriffer-Hegger (SSH) model describing an atomic lattice with stagger hopping integrals. 21–23 The SSH system is characterized by two different phases (with or without topological end states), which are topologically distinct. These states are protected against external disturbances. 24 The experimental realization of the SSH model is based on optical lattices or on the real atomic lattice (with vacancies) in a chlorine monolayer surface. 25–27

Freely suspended chains of metallic atoms fabricated, e.g., in the mechanically break junction method 28–30 are relatively short and can easily break, which make these structures useless from the practical point of view. On the other hand, very stable atomic chains can be grown epitaxially on reconstructed silicon surfaces [like Si(335), Si (557), or others]. 1–4,28 Such single atomic chains or atomic ribbons are coupled with the surface leading to electron leakage to the substrate states and asymmetry in the density of states (DOS). 27,28 Thus, electron localization in the substrate can significantly modify electronic properties of atomic ribbons. Particularly interesting are low-dimensional conductors with spin–orbit coupling, 29–32 where spin-polarized currents can appear (local asymmetric confinement of electrons leads to spin-orbit coupling of Rashba type). 24 The asymmetrical potential produces the precession of electron spins, which is responsible for spin-flip scattering between neighboring sites in the ribbon. Phonon interactions, magnetic impurities, or nuclear spins can lead to the on-site spin-flip processes. 33 Although there are many papers on the spin–orbit systems, very little attention has been paid to investigate the role of the substrate coupled with spin-orbit chains, ...
where the electron localization effects can be very important. It makes the model more realistic and interesting as the chain-substrate systems reveal new physical properties (superradiant states, asymmetry in DOS, and ferromagnetic occupancies). They can be useful in spintronics, e.g., as spin–orbit qubits, spin pumps, or basic elements of spin transistors.30,36 The spin-orbit coupling strength can be experimentally tuned by external gates and can lead to oscillatory behavior of the ballistic spin conductance.32,37

In this paper, we are focusing on the electrical properties of normal and topological atomic chains (ribbons) on different substrates taking into account the spin-orbit scattering. Electron localization in the substrate introduces asymmetry in DOS (Dicke-like effect) but does not mix spin states. On the other hand, the spin-orbit interactions break spin symmetry in the system and thus, it is a great challenge to investigate electrical properties of atomic ribbons in the presence of both surface scattering and spin-orbit couplings. They together can lead to paramagnetic or ferromagnetic solutions with nonsymmetrical spin-dependent DOS and asymmetrical (or irregular) electron occupancies along the atomic ribbon. In our calculations, we consider the spatial separation of atoms and use the substrate model, which allows us to consider the insulator (strongly localized electrons in the substrate), the semiconductor, as well as metallic surfaces (delocalized electrons in the substrate).27,38

We analyze the asymmetry in the local DOS, DOS at the Fermi level, and the electron occupancies along the system for normal and SSH topological chains. The results of this paper give some insight into the physics of end states, charge density waves (CDW), Friedel oscillations, and topological states in quasi-1D systems. The careful inspection of the local DOS (which is possible using spin-polarized STM), topological states, or charge waves can provide useful information about the hopping amplitudes, on-site single-electron energies, and the ribbon geometry. In our studies, we propose long atomic chains on a substrate as a memory storage device fully controlled by the surface and spin-orbit coupling parameters.

The paper is organized as follows. In Sec. II, we describe the theoretical model and the calculation method for the tight-binding Hamiltonian. In Sec. III, the main results of the paper are discussed: for short atomic systems (Sec. III A), for normal and SSH single atomic chain (Sec. III B–III D), and for coupled chains (ribbons), (Sec. III E). Section IV gives a short summary.

II. MODEL AND THEORETICAL DESCRIPTION

The elementary system we consider in this paper is schematically shown in Fig. 1. It consists of $M$ linear atomic chains (each composed of $N$ sites, red balls) coupled with the substrate electrode. The system corresponds to atomic ribbons, which can be fabricated on stepped-like, vicinal surfaces.14 The model tight-binding Hamiltonian for this system includes the spin-flip and spin–orbit couplings and can be written in the following form: $H = H_0 + H_\alpha$, where

$$H_0 = \sum_\sigma \left( \sum_{i=1}^{N\cdot M} E_{i\sigma} a_{i\sigma}^\dagger a_{i\sigma} + \sum_k E_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma} \right)$$

$$+ \sum_{(ij)} t_{ij} a_{i\sigma}^\dagger a_{j\sigma} + \sum_{k,l} V_{k\alpha\sigma} a_{i\sigma}^\dagger c_{k\sigma}^\dagger + \text{h.c.},$$  

(1)

describes the on-site electron energies in the atomic ribbon, $E_{i\sigma}$ ($i = 1, \ldots, N \cdot M$), with spin $\sigma$, and the electron energies in the substrate with the wave vectors $\tilde{k}$, $E_{\tilde{k}\sigma}$. The operators $a_{i\sigma} (a_{i\sigma}^\dagger)$ annihilate and create an electron with spin $\sigma$ at the $i$-th site, and $c_{k\sigma} (c_{k\sigma}^\dagger)$ are the according substrate operators (related to the substrate Bloch states). Electron transition between neighboring states in the ribbon is described by $t_{ij}$ elements (here $(i,j)$ means the summation over the neighboring sites) and for regular chains, like, e.g., Pb atoms on Si(111) vicinal surfaces, this parameter is spin and position independent and we can take $t_{i\pm 1} = t_i$ (along each chains) and $t_{i\pm N} = t_N$ (between chains). For nonuniform couplings, along the chains, $t_{ij}$, e.g., for different every second couplings, the system corresponds to the topological SSH chain19,21 which will be considered later. The last term of $H_\alpha$ represents electron hybridization of the ribbon states with the substrate Bloch states which in general depends on site positions, $R_i$ (i.e., spatial separation of atoms are considered): $V_{i\alpha\sigma} = V_\alpha \exp(i k R_i)$, and here is spin-independent. Thus, the spectral density matrix can be written as follows: $\Gamma_S = 2 \pi \sum_{k} V_{\tilde{k}\alpha\sigma} V_{\tilde{k}\sigma\alpha}^\dagger \delta(E - E_{\tilde{k}})$. Assuming that only the substrate electrons close to the Fermi surface play an important role and for equal distances between atomic sites in the ribbon, $a$, one obtains $\Gamma_S = \Gamma_S \delta(E - e_F)$, where $\Gamma_S = \langle \Gamma_S \rangle = 2 \pi \sum_{k} |V_{\tilde{k}\alpha\sigma}|^2 \delta(E - E_{\tilde{k}})$ stands for the effective atom-substrate coupling strength, which in the wide band limit is energy independent. Here, $r_{ij}$ is the distance between two atomic sites in the ribbon, $r_{ij} = |R_i - R_j|$, and is expressed in $a$ units, thus for two sites from the same chain $r_{ij} = |j - i|$, but in general, it should be obtained from the Pythagorean theorem. The parameter $k_{\sigma\alpha}$ in the above relation is responsible for the electron localization in the substrate. For very small $k_{\sigma\alpha}$, all elements of the spectral density matrix $\Gamma_S$ are position independent and in this case (for $k_{\sigma\alpha} = 0$), we have $\langle \Gamma_S \rangle = \Gamma_S$. In this limit, an electron from the ribbon can flow to the substrate, and then it can appear at the arbitrary site with the same probability. It corresponds to delocalized electron states in the substrate, which is satisfied for metallic-like surfaces. In the opposite limit, for very large value of $k_{\sigma\alpha}$, the spectral density matrix is diagonal and for $k_{\sigma\alpha} = \infty$, one finds $\langle \Gamma_S \rangle = \Gamma S \delta p$. In this case, each ribbon site is coupled effectively to an individual electrode and an electron that
tunnels from a particular site to the substrate can re-enter only at the same site. This limit describes localized electrons in the substrate with very short mean-free path, which corresponds to semiconductor or insulator substrates.

The spin–orbit couplings can be effectively modelled by spin-flip hopping terms in a usual tight-binding approach.\(^\text{17,25,27}\) In this treatment, the spin-orbit Hamiltonian is composed of spin-flip processes at a given site and between neighboring sites and can be written in the following form:

\[
H_{\text{so}} = \sum_{\sigma \sigma'} \left( t^{i \alpha}_{\sigma} \sum_{j} a^{\dagger}_{\sigma j} (\mathbf{\sigma} \cdot \mathbf{r}_{ij}) a_{\sigma' j} \right)
- t^{i \alpha}_{\sigma} \sum_{j} a^{\dagger}_{\sigma j} (\mathbf{\sigma} \cdot \mathbf{r}_{ij}) a_{\sigma' j} + \sum_{\sigma \sigma'} t^{i \alpha}_{\sigma} a^{\dagger}_{\sigma j} a_{\sigma' j} + \text{h.c.},
\]

where \(\mathbf{\sigma} = (\sigma_x, \sigma_y, \sigma_z)\) are the Pauli matrices and \(\sum_{\alpha \beta} \) corresponds to summation over the neighboring sites within a given atomic chain, and \(\sum_{\alpha \beta} \) between neighboring sites from different atomic chains.

Here, we consider the system where many-body effects (like the Kondo effect) do not play an important role and they can be omitted in the Hamiltonian. In this sense, the electron-electron interactions is captured by an effective shift of the on-site energies, \(\varepsilon_{ij}\), which is reasonably well satisfied for many atoms (like Au, Ag, In, or Pb) on vicinal silicon surfaces.\(^\text{28,29}\) In our calculations, we concentrate on the local DOS at a given site, the local DOS at the Fermi level, and the electron occupancies along the ribbon. These quantities can be found from the knowledge of retarded Green functions, \(G_i^R\), corresponding to the appropriate ribbon sites. Using the equation of motion for retarded Green’s function\(^\text{30}\) together with the Hamiltonian one can obtain \(2(N \times M)\) linear-dependent equations for the retarded Green’s function elements, \(G_i^R(E)\). They can be written in the matrix notation \(G^R = C^I I^R\), where \(I^R\) is the identity matrix and \(C\) is a square \((2N \times M) \times (2N \times M)\) complex array, which inverse stands for the Green’s function. This function can be obtained from the relation \(G^T C = \text{det} C\), where \(\text{det} C\) is the \((i,j)\) cofactor of \(C\) matrix. From the knowledge of retarded Green’s function, we obtain the local DOS (LDOS) at the \(i\)-th site, \(\text{LDOS}(E) = - \frac{1}{\pi} \text{Im} G_i^R(E)\), and the electron occupancy \(n_i = \frac{1}{\pi} \text{Im} \text{LDOS}(E) dE\).

Now, we specify \(C\) matrix corresponding to coupled atomic chains on the substrate. It can be written in the following form:

\[
\hat{C} = \begin{bmatrix} \hat{A}^\sigma(E) & \hat{D}^\sigma(E) \\ \hat{D}^\sigma(E) & \hat{A}^{-\sigma}(E) \end{bmatrix}.
\]

Each submatrix of \(\hat{C}\) has a dimension of \((N \times M) \times (N \times M)\). Let us first describe diagonal matrices of \(\hat{C}, \hat{A}^\sigma(E)\). They are composed of the following submatrices:

\[
\hat{A}^\sigma(E) = \begin{bmatrix} \hat{B}_{II} & \hat{B}_{II} & \hat{B}_{II} & \ldots \\ \hat{B}_{II} & \hat{B}_{II} & \hat{B}_{II} & \ldots \\ \hat{B}_{II} & \hat{B}_{II} & \hat{B}_{II} & \ldots \\ \hat{B}_{M} & \hat{B}_{M} & \hat{B}_{M} & \hat{B}_{M} \end{bmatrix},
\]

where \(\hat{B}_{\alpha \beta}\) concerns the square matrix related to all sites from \(\alpha\) and \(\beta\) rows (\(\alpha, \beta = I, \ldots, M\)) with spin \(\sigma\) [or with spin \(-\sigma\) for \(A^{-\sigma}(E)\) matrix]. For \(\alpha = \beta\), it takes the following form:

\[
(\hat{B}_{\alpha \alpha})_{ij} = (E - \varepsilon_i) \delta_{ij} - t_{ij+1} (\delta_{ij+1} + \delta_{ij-1}) + i \left( \frac{\Gamma_j}{2} \right).
\]

For the neighboring \(\alpha\) indexes (upper and lower diagonal submatrices of \(\hat{A}\)), \(\hat{B}\) can be written as follows:

\[
\hat{B}_{\alpha \alpha \pm M} = -t_{ij} \delta_{ij} + i \frac{1}{2} \Gamma_j^2,
\]

and for other indexes: \(\hat{B}_{\alpha \beta} = i \frac{1}{2} \Gamma_j\). Now, we describe off-diagonal elements of \(\hat{C}\) matrix, which are related with the spin-orbit couplings (electron states with different spins), \(\hat{D}^\sigma(E)\). In general, this matrix is tri-diagonal and is composed of \(\hat{E}\) submatrices

\[
\hat{D}^\sigma(E) = \begin{bmatrix} \hat{E}_{II} & \hat{E}_{II} & 0 \\ \hat{E}_{II} & \hat{E}_{II} & \hat{E}_{II} \\ 0 & \hat{E}_{II} & \hat{E}_{II} \end{bmatrix},
\]

where the diagonal submatrices describe spin-flip and spin-orbit couplings along the chains and take the form \((\hat{E}_{\alpha \alpha \pm M})_{ij} = -t_{ij} \delta_{ij} - t_{ij}^{\pm} (\delta_{j-1} - \delta_{j+1})\). The upper and lower diagonal submatrices of the above matrix are related to spin-orbit couplings between chains and are diagonal complex matrices \(\hat{E}_{\alpha \alpha \pm M} = \mp i t_{ij} \delta_{ij} \). Other elements of \(\hat{D}\) are zero. Note that due to complexity of \(\hat{A}\), it is difficult to find the short analytical form of \(\hat{G}\). However, some analytical results exist for the linear geometry of the system (left lead–chain–right lead), where only tri-diagonal matrices appear and their determinates can be expressed by the Chebyshev polynomial of the second kind.\(^\text{31}\) In this paper, we discuss some analytical calculations for short atomic chains.

### III. RESULTS AND DISCUSSION

In our calculations, the temperature is \(T = 0\) K, and the energy reference point stands for the Fermi energy of the substrate, \(E_F = 0\). It is assumed that each atomic site in the ribbon couples equally strong to the substrate independently on spin, \((\Gamma_j)_{\alpha \alpha} = \Gamma_j\), which is the energy unit. Moreover, only regular atomic chains are considered, i.e., the on-site electron energies as well as the intra-chain couplings are position and spin independent, \(\varepsilon_{ij} = \varepsilon_i\), \(t_{ij}^\pm = t_{ij}^\alpha = t_{ij}\) and \(t_{i,i+1} = t_i\) (between the neighboring sites along each chain) and \(t_{i,i+N} = t_i\) (between neighboring sites from different chains). These assumptions are quite reasonable for regular chains consisting of one atom species in an equidistant arrangement on the surface like Pb on the Si(553)/Au substrate. The parameters of the system have been used in order to satisfy the realistic situation in many experiments, e.g., assuming \(\Gamma_j = 0.25\) eV, the hopping integral along the chain is \(t_i = 4 = 1\) eV, between chains is \(t_p = 2 = 0.5\) eV, spin-orbit and spin-flip couplings, \(t_{io/\delta} = 0.1 = 25\) meV, cf. Refs. 4, 27, 32, and 35.

### A. Short atomic systems

In this subsection, we analyze the role of the substrate and spin-orbit couplings on the electronic properties of short atomic...
systems. It allows us to find the main modifications of the local DOS due to spin-orbit couplings and to better understand the properties of larger systems and atomic ribbons.

For a chain composed of two coupled atoms on the substrate, one finds that

\[ \hat{\mathcal{A}}^\sigma(E) = \begin{bmatrix} E - \varepsilon_{i\sigma} + i\frac{\Gamma_{i\sigma}}{2} & -t_{k} + i\frac{\Gamma_{k\sigma}}{2} \\ -t_{k} + i\frac{\Gamma_{k\sigma}}{2} & E - \varepsilon_{j\sigma} + i\frac{\Gamma_{j\sigma}}{2} \end{bmatrix}, \]

and the determinant of \( \hat{\mathcal{C}} \) matrix equals \( \det \hat{\mathcal{C}} = \det(\hat{\mathcal{A}}^\sigma - \hat{\mathcal{D}}^\sigma) \) \( \det A^{-\sigma} \), where \( \det A^{\pm \sigma} \) for arbitrary \( N \) and no substrate \( (\Gamma_z = 0) \) can be obtained analytically.\(^{40,41} \)

For \( t_{k0} = 0 \), one can write \( \det \hat{\mathcal{C}} = \det(\hat{\mathcal{A}}^\sigma - \hat{\mathcal{D}}^\sigma)^{-1} \) \( \det A^{-\sigma} \). For the case of \( t_{gf} = 0 \) and \( t_{k0} \neq 0 \), we have \( \det \hat{\mathcal{C}} = \det(\hat{\mathcal{A}}^\sigma - \hat{\mathcal{D}}^\sigma)^{-1} \) \( \det A^{-\sigma} \), and similar relations one can write for the cofactor of \( \hat{\mathcal{C}} \). Note that for nonzero spin-flip and spin-orbit couplings, one can obtain analytically all Green’s function elements but the relations for LDOS or on-site occupancies cannot be written in relatively simple and transparent forms, and thus we skip them in the paper.

In Fig. 2, we consider a two-atom system on a substrate and study the role of the spin-flip and spin-orbit couplings on the local DOS for both spins \( \sigma \) and \( -\sigma \) (red solid and blue broken curves, respectively). Such a system for \( t_{k0} = t_{gf} = 0 \) is characterized by two local maxima of LDOS localized exactly at \( E = \varepsilon_{0} \pm t_{k} \) (not shown here) and the local DOS is spin-independent in this case. In the presence of the spin-orbit coupling (upper panel), these maxima of LDOS move outside a little and appear at \( E = \varepsilon_{0} \pm t_{k} \), but the symmetry of LDOS around \( E = \varepsilon_{0} \) is still visible. For nonzero spin-flip coupling, \( t_{gf} \) (and \( t_{k0} = 0 \), middle panel), the structure of LDOS is still spin-independent (red solid and blue broken curves overlap each other) and is symmetrical around \( E = \varepsilon_{0} \), but each maximum of DOS splits into two local peaks separated by \( 2t_{gf} \). Thus, in this case, one observes four local maxima of LDOS localized at \( E = \varepsilon_{0} \pm t_{k} \). Note that for \( t_{gf} = t_{gf} \), only three local maxima appear in the structure of LDOS. The situation changes in the presence of both spin-flip and spin-orbit couplings (bottom panel) as in this case, the local DOS at each atomic site depends on spin and in general, \( \text{LDOS}_{\sigma}(E) \neq \text{LDOS}_{-\sigma}(E) \). This spin-asymmetry results from the fact that the spin-flip transition between the sites \( |1\sigma> \rightarrow |2 - \sigma> \) is not the same as for \( |1 - \sigma> \rightarrow |2\sigma> \) (cf. also \( D \) matrix). It can also be confirmed analytically: \( G \) is obtained from the knowledge of \( \text{cof} \hat{\mathcal{C}} \) and \( \det \hat{\mathcal{C}} \), here the determinant of \( \hat{\mathcal{C}} \) is the same for both spins; however, the cofactor of \( \hat{\mathcal{C}} \) is spin-dependent. For our system, one can obtain that the difference of both cofactors for spin up and spin down equals

\[ (\text{cof} \hat{\mathcal{C}})_{1\sigma,1\sigma} - (\text{cof} \hat{\mathcal{C}})_{1,1\sigma} = 4t_{gf}t_{gf} \left( t_{gf} + \frac{\Gamma_{1\sigma}}{2} \right). \]

It means that for \( t_{gf} = 0 \) or \( t_{gf} = 0 \), there is no difference between both cofactors, and thus the local DOS is spin independent, while for nonzero both \( t_{gf} \) and \( t_{k0} \), the cofactor difference leads to spin dependence of LDOS. Note that due to spin-orbit couplings, the local DOS at the second site for a given spin is not the same as at the first site but corresponds to the opposite spin, i.e., \( \text{LDOS}_{\sigma}(E) = \text{LDOS}_{-\sigma}(E) \) and \( \text{LDOS}_{-\sigma}(E) = \text{LDOS}_{\sigma}(E) \). It is also important that the structure of spin-dependent LDOS is non-symmetrical vs the Fermi energy, which leads to different occupancies for both spins and will be studied later. However, the total DOS at each atomic site [obtained as \( \text{LDOS}_{\sigma}(E) + \text{LDOS}_{-\sigma}(E) \)] is fully symmetrical (black-dotted curve in Fig. 2, bottom panel). The asymmetry in the local DOS structure which appears in the presence of spin-flip and spin-orbit couplings, can be detected using spin-polarized electron leads (e.g., in STM experiments). For a normal STM electrode, where both electron spins are present...
simultaneously, one cannot distinguish between LDOS signals from each spin and the results are always symmetrical.

Real atomic chains or atomic clusters are often fabricated on different substrates (metallic, semiconductor, or insulator), thus it is desirable to investigate the role of the \( k_\text{fl} \) parameter on the local DOS in the presence of spin-flip and spin-orbit couplings. In Fig. 3, we show the local DOS for both spins at the first atomic site for small \( k_\text{fl} \) (upper panels) and for larger \( k_\text{fl} \) (bottom panels). Additionally, we consider the system with the spin-orbit couplings (right panels) and for \( t_\text{ff} = t_\text{so} = 0 \) (left panels). In the last case, the LDOS curves are spin-independent. As one can see for small value of \( k_\text{fl} \), the structure of LDOS is nonsymmetrical for both \( t_\text{ff} = t_\text{so} = 0 \) and \( t_\text{ff} = t_\text{so} = 1 \). This asymmetry is a hallmark of the Dicke-like peak and a wide smooth background (for \( k_\text{fl} = 0 \), \( k_\text{fl} = 0.1, 0.2, \) and \( 0.3 \) respectively, for better visualization). In our case, both atomic sites are coupled with continuum states of the substrate and the spectral functions of these atoms are characterized by two peaks: a wide Lorentz-like peak and a very narrow Dicke peak, see also Refs. 28 and 43. For \( t_\text{ff} = t_\text{so} = 0 \) (left panels), LDOS asymmetry vanishes with increasing \( k_\text{fl} \). For \( k_\text{fl} = 4 \), LDOS is still asymmetrical but for fully localized electrons in the substrate, \( k_\text{fl} \rightarrow \infty \), the structure of LDOS is perfectly symmetrical as in this case \( \langle \Gamma \rangle_{ij} = \delta_i \Gamma_j \). In the presence of spin-flip and spin-orbit couplings, \( t_\text{ff} = t_\text{so} = 1 \), one observes that each LDOS peak splits (cf. the left and right panels). Moreover, the results are spin-dependent even for larger values of \( k_\text{fl} \) (see also Fig. 2, bottom panel obtained for \( k_\text{fl} = 10 \)).

The results analyzed in this subsection indicate that there are two reasons for asymmetry in LDOS for atomic systems: localized electrons in the substrate and spin-orbit couplings. The former is spin-independent, and the latter depends on spins. Thus, it is interesting to consider these effects for larger systems taking into account partially localized substrate electrons in the presence of spin-flip and spin-orbit couplings which we study below.

B. Atomic chains on different substrates

In small atomic systems, in the absence of spin-orbit couplings, we have observed strong asymmetry in LDOS for delocalized electrons in the substrate and almost symmetric LDOS for localized surface electrons. On the other hand, for nonzero spin-orbit couplings, the local DOS curves are always nonsymmetrical for both regimes of the \( k_\text{fl} \) parameter. In this subsection, we study how the surface electrons modify the structure of LDOS for regular atomic chains taking into account the system with and without spin-flip and spin-orbit couplings.

In Fig. 4, we analyze the local DOS at the middle site of the atomic chain composed of 50 sites for different values of \( k_\text{fl} \) and \( t_\text{so} = t_\text{fl} = 0 \). For small \( k_\text{fl} \) (upper curve), one observes large number of LDOS peaks related to \( N \) sites, but the structure of LDOS is nonsymmetrical. For larger, intermediate \( k_\text{fl} \) (partially localized electrons), these LDOS peaks are still visible for negative energies, and for positive ones, the LDOS curve is smoother. Finally, the structure of LDOS is characterized by a single Dicke-like peak and a wide smooth background (for \( k_\text{fl} = 3 \))—such a structure is similar to that one obtained for \( N = 2 \) (Fig. 3, left upper panel). For larger and larger \( k_\text{fl} \), the Dicke peak vanishes and the local DOS is symmetrical with no localized peaks (bottom curve). The appearance of peaked-like DOS together with the smooth DOS for the intermediate values of \( k_\text{fl} \) influences the electron occupations along the chain and will be studied later.

Note that in the absence of spin-orbit couplings, the LDOS curves are spin-independent for all atomic sites in the chain. The situation can change for nonzero \( t_\text{so} \) and \( t_\text{fl} \) parameters. Thus, in Fig. 5, we consider atomic chains with the spin-flip and spin-orbit coupling...
couplings and investigate the role of electron localization in the substrate on the local DOS. We show the results for $k_F a = 1.5$ (upper panels) and $k_F a = 3$ (bottom panels) and analyze the structure of LDOS at the chain end ($i = 1$, left panel) and in the middle of the chain ($i = 25$, right panels). As one can see the structure of the local DOS is asymmetrical and splits, leading to a wider energy region of nonzero LDOS with two spin-degenerate Dicke peaks for intermediate $k_F a$ parameter (separated by $2t_f$), right bottom panel. More important, the local DOS is almost spin-independent, blue and red curves overlap (right panels). It is in contrast to our previous results from Fig. 3 for the two-atom system and nonzero $t_{so}$ and $t_f$. To study this problem in a wider context, we also plot the local DOS at the first chain site for both spins (left panels) and find that at both chain ends, the electron spectral function depends on spin. Moreover, this function does not reveal Dicke peaks and is nonasymmetrical. Thus, we have found that in the presence of the spin-flip and spin-orbit couplings, both chain ends show spin-dependent DOS characteristics, whereas in the middle of the chain, only paramagnetic solutions are realized with almost spin-independent local DOS. This feature of linear atomic chains on a substrate has a strong influence on their electrical properties and suggests that the nonmagnetic chain can be spin polarized. However, spin-memory cells can be localized only at both chain ends.

C. Charge distribution and LDOS oscillations

The structure of LDOS analyzed in Sec. III B is crucial for electron occupations of atomic sites, which are related to spin-polarized charges and spin-transport properties. To corroborate the existence of spin-dependent occupations at both chain ends in Fig. 6, we study electron charges along the chain composed of $N = 50$ sites as a function of the electron localization parameter, $k_F a$. As one can see for small $k_F a$, the occupancies increase because the local DOS peaks move below the Fermi energy, cf. Fig. 4. Then, one observes two local maxima of $n_{i\sigma}$, which are related to the split structure of LDOS showed in Fig. 5, right panels, with two Dicke-like peaks. For larger $k_F a$, the local DOS is smoother and smoother and the site occupancies monotonically decrease. Note that the Friedel oscillations with the period of two atoms appear only at both chain ends. These oscillations decrease with $k_F a$ and are not observed in the middle of the chain, as expected.

It is worth noting that without spin-flip and spin-orbit couplings, charge distribution along the chain is always symmetrical, i.e., $n_{i\sigma} = n_{i-1\sigma}$. However, in the presence of the spin-orbit couplings (Fig. 6), the occupancies along the chain are different at both chain ends and $n_{i\sigma} \neq n_{i-1\sigma}$. This effect is analyzed in the bottom panel, where we show the occupancies for both spins at each atomic site. The asymmetry in $n_{i\sigma}$ along the chain is related to the nonsymmetrical structure of the local DOS in the presence of the spin-flip and spin-orbit couplings. As a main feature of our atomic chain, we have found that the occupancies along the system are spin-dependent only at both chain ends, where spin-dependent Friedel oscillations appear. In the middle of the chain, the occupancies are spin-independent and only paramagnetic solutions are observed, $n_{i\sigma} = n_{i-\sigma}$. Thus, only chain ends can store spin-dependent information.

The oscillations of occupancies along the chain should be also reflected in the structure of the local DOS at the Fermi level, which is often measured in the STM experiments. Thus, in Fig. 7, we study the local DOS along the atomic chain composed of $N = 50$ linear sites for different spin-flip and spin-orbit parameters.
upper panel, we consider \( t_{sf} = 0 \) and show the results for \( t_{so} = 0.1 \) and 1. The local DOS is characterized by a relatively flat structure with even-odd Friedel oscillations at both chain ends, which are more evident for larger \( t_{so} \) (broken curve). The situation changes in the presence of nonzero spin-flip parameter, \( t_f \) (and for \( t_{so} = 0 \), middle panel). Note that the \( t_f \) parameter is responsible for splitting of the local DOS peaks, which can effectively change the positions of the on-site energies, \( \varepsilon_0 \). Thus, for small \( t_f \), the modified even-odd oscillations are visible along the chain (middle panel, lower curve). For larger \( t_f \), the positions of split LDOS peaks move and they can satisfy the condition for the conductance oscillations. The period of these oscillations is determined by the relative position of the effective on-site energy levels, \( \varepsilon_{eff} \), the Fermi energy, \( E_F \), and the coupling parameters: \( \cos(\frac{\pi}{m}) = \frac{k_F a}{E_F - \varepsilon_0} \), where \( m \) is the oscillation period and \( i = 1, \ldots, m - 1 \). Here, for \( t_f = 1 \), regular nonvanishing DOS oscillations with the three-atom period are observed as in this case, a single atomic site is characterized by two LDOS peaks at \( E = \pm t_g \), and for \( t_f = t_s \), it corresponds to the condition for the conductance oscillations with the period of 3 atoms (\( \varepsilon_{eff} = \pm t_s \)). For larger \( t_g \), the oscillation amplitude changes and LDOS oscillations become irregular. In the presence of both spin-flip and spin orbit couplings (bottom panel), one observes slightly even-odd oscillations for small \( t_{so}, t_f \) (solid red curve), and regular oscillations of LDOS with the period of about 6 atoms for larger couplings (broken blue curve). This period comes from a superposition of the even-odd period (upper panel, \( m = 2 \)) and the three-atom period (middle panel, \( m = 3 \)) indicated by the blue-dotted curves. Note that all curves from the upper and middle panels are fully symmetrical along the chain, but for nonzero spin-orbit and spin-flip couplings (bottom panel), the local DOS along the chain depends on the electron spin and is non-symmetrical, which is especially visible at both chain ends (cf. also the asymmetry in Fig. 2 for the two-atom system). For strongly localized electrons in the substrate, \( k_F a \rightarrow \infty \), the local DOS oscillations along the chain vanish leading to only small even-odd oscillations at both chain ends. The above results show that the spin-orbit and spin-flip couplings can effectively modify charge distribution (periods and amplitudes) along the chain.

D. SSH spin-orbit chains

In this subsection, we consider the SSH chain in the topological phase with the spin-orbit and spin-flip couplings. We expect that paramagnetic occupancies inside the chain as well as charge distribution along the chain will be enhanced in the presence of topological end states. Topological states in the SSH model appear at both chain ends for different (but regular) couplings along the chain—here, we set \( t_{i+1} = 2 \) (for odd \( i \) and \( t_{i+1} = 4 \) (for even \( i \)), which in the short form can be written as \( t_s = 2, 4 \). It leads to the energy gap inside the chain for the energy region \( E = \varepsilon_0 \pm 2 \).

In Fig. 8, we analyze the local DOS at the first atomic site of the chain and compare these results with the corresponding ones for the middle site of the chain, left and right panels, respectively. As one can see for no spin-flip and spin-orbit couplings, the chain is characterized by a topological state at the first atomic site which is spin-independent (left upper panel, solid red and broken blue curves) or by an energy gap in the local DOS inside the chain (right upper panel). It is worth mentioning that in the literature, the SSH chain is mostly considered in the linear geometry (the chain is coupled with the left electrode via the first atomic site and with the right one via the last site). In such a configuration, the local DOS exhibits strong oscillating (peaked) structure—see the broken black curves in the upper panels, but the topological state at \( i = 1 \) as well as the energy gap inside the chain appear for the same energies. For the geometry considered in this paper, each atomic site of the chain is coupled with the surface and their spectral functions are more smoother than for the mentioned linear geometry. Note very symmetrical structures of LDOS around \( E = \varepsilon_0 \) for both configurations as we consider here almost localized electrons in the substrate.

In the presence of the spin-flip and spin-orbit couplings in the SSH chain, bottom panels, the local DOS is spin-dependent (the solid red and broken blue curves do not cover each other) and the symmetry of the local DOS is broken. One should notice that the topological state at the first atomic site (which appears in the middle of the energy gap region) splits leading to asymmetry in LDOS and two local maxima are observed (left bottom panel). Thus, one should observe ferromagnetic occupancies at both ends of the SSH chain.
However, for the SSH chain, all sites are characterized by nonsymmetrical LDOS (cf. right bottom panel for $i = 25$), which leads to spin-polarized solutions inside the chain.

To corroborate this effect, we obtain the electron occupancies along the SSH chain (bottom panel in Fig. 9) and compare them with the occupancies for the normal chain (upper panel). Note that for no spin-flip and spin-orbit couplings, the occupancies do not depend on spin (only paramagnetic solutions are realized) and do not depend on the chain topology (see the blue-dotted curve in the bottom panel obtained for the SSH chain for $t_f = t_0 = 0$). In the presence of the spin-orbit terms, spin-polarized occupancies are possible. However, in normal chains (upper panel), paramagnetic occupancies dominate inside the chain and only both chain ends are spin-polarized. The situation changes for topological SSH chains, where we observe oscillations of the electron occupancies along the whole chain (bottom panel).

It is very important in the context of the Friedel oscillations, which are strongly damped in the SSH chains due to an energy gap at the Fermi level.34 However, in our case, for spin-orbit SSH chains, we have found spin-dependent (and nondumped) oscillations of $n_{\sigma \sigma}$. These oscillations are very regular inside the chain with some disturbances at both chain ends, where topological states are localized. Moreover, the occupancies are spin-polarized along the whole SSH chain, which was not observed for normal chains, and they are asymmetrical, $n_{\sigma \sigma} = n_{(N-i+1)-\sigma}$. It is interesting that although we observe oscillations of $n_{\sigma \sigma} \neq n_{-\sigma-\sigma}$ along the chain the average electron occupancies at each site, $\overline{n_{\sigma \sigma} + n_{-\sigma-\sigma}}$, do not oscillate at all and overlap with the blue line for $t_f = t_0 = 0$ in the bottom panel. It means that spin-dependent Friedel oscillations in the SSH chain can be detected using spin-polarized external electrodes. The results described above allow one to control chain polarization by means of spin-orbit parameters or by means of topology parameters (the coupling strengths). In this sense, we can use such SSH chains to store and control quantum information in 1D atomic systems.

E. Atomic ribbons

Single atomic chains are the thinnest possible electric wires but are prone to external perturbations or defects and can be unstable. More solid structures on the substrate are coupled atomic chains. In this section, we analyze LDOS oscillations along atomic ribbons on different surfaces with the spin-orbit and spin-flip couplings. First, we consider two-chain ribbon for $t_f = t_0 = 0$ (upper panel in Fig. 10). As one can see, for decoupled chains in the ribbon, $t_r = 0$, the Friedel even-odd oscillations of LDOS are visible at both chain ends; however, for coupled chains, $t_r = 1$, the local DOS oscillates with the period of three sites. In the last case, nonzero couplings between chains lead to renormalization of the on-site energies at atomic sites and if these effective energies satisfy the condition on the conductance oscillations, one observes the oscillations of LDOS along the chain with the same period as the conductance oscillations.44 Of course, the spin-orbit as well as the spin-flip couplings also change the energy of on-site states and split these states, which can modify the oscillation period of LDOS. Such a case is shown in the middle panel for two-chain ribbon in the presence of spin-flip coupling (blue broken curve with crosses).
or in the presence of spin-orbit coupling (pink-dotted curve with rectangles). In the former case \((t_{sf} \neq 0, t_{so} = 0)\), the on-site electron energies are split leading to oscillations of LDOS with the period of 5–6 atomic sites, whereas in the latter case (for \(t_{so} \neq 0, t_{sf} = 0\)), the energies of atomic states move in the energy scale and their new positions generate the oscillations period of 4 sites in the system. The most interesting case is shown in the bottom panel in Fig. 10, where we analyze the local DOS along the double-chain ribbon in the presence of both spin-flip and spin-orbit couplings. Now, the oscillation period of LDOS is a combination of the periods from the middle panel and equals about 15 atomic sites. It is worth noting that the local DOS along the ribbon is the nonsymmetrical function only in the last case, i.e., for \(t_{sf} \neq 0, t_{so} \neq 0\) (bottom panel). For other cases, all LDOS curves are fully symmetrical along the ribbon and are spin-independent. We have shown that the period and the intensity of the LDOS oscillations along the atomic ribbon can be controlled by coupling parameters.

The results shown in Fig. 10 were obtained for only one (intermediate) \(k_F a\) parameter. In our further studies, we are going to investigate the role of the electron localization in the substrate on the LDOS oscillations along the atomic ribbon. Thus, in Fig. 11, the local DOS along the double-chain ribbon is shown as a function of the electron localization parameter, \(k_F a\), in the presence of both spin-orbit and spin-flip couplings. One can distinguish here two regimes of \(k_F a\). For small value of this parameter (delocalized electrons in the substrate) the local DOS changes irregularly with \(i\) but for somewhat larger values of \(k_F a\), the oscillations become very regular with the period of about 15 sites (cf. also the bottom panel in Fig. 10). The appearance of almost flat and site-independent \(\text{LDOS}(E_F)\) for larger \(k_F a\) is related with modifications of the spectral density function due to the presence of the substrate which was analyzed in Figs. 4 and 5 for a single atomic chain. In that case the corresponding local DOS becomes flat around the Fermi energy, which makes the system less interesting for potential applications.

In the last studies of this paper, we consider a wider atomic ribbon and analyze three coupled chains on a substrate. For two coupled chains, the results along the first or the second chain were always the same. For wider ribbons, we expect that the results can differ from row to row of atoms. In Fig. 12, we consider a ribbon composed of three coupled chains, \(t_i = 1\), for very small spin-orbit coupling, \(t_{sf} = t_{so} = 0.1\) (upper panel), and for \(t_{sf} = t_{so} = 0.2\) and 0.5 (middle and bottom panels). For the chosen set of parameters, the local DOS oscillates with the period of 4-sites with a relatively large amplitude (upper panel). Moreover, these oscillations are exactly the same for rows I and III (red solid line and black dots) and slightly differ for row II (larger oscillation amplitude). Note that the minima and maxima of the local DOS oscillations are in phase for each atomic row. For somewhat larger spin-orbit couplings (middle panel), the oscillations of LDOS become irregular but still they are in phase for considered rows of atoms. For larger spin-orbit couplings (bottom panel), the oscillation amplitudes decrease and regular oscillations are still visible, but more important, the results for the middle chain and for both side chains are out of phase, i.e., the minima of LDOS for row II correspond to maxima of I and III chains. Additionally, asymmetry in the structure of the local DOS appears at both ribbon ends for each atomic row (similarly to the results presented for the two-atom system and the for atomic chain). This effect is better visible for larger spin-orbit couplings and leads to ferromagnetic occupancies of
edge sites and paramagnetic ones inside the ribbon. The asymmetry of LDOS in the ribbon and out-of-phase oscillations of the local DOS along different ribbon chains can be confirmed experimentally in the STM experiments.

IV. CONCLUSIONS

We have studied electronic properties of atomic ribbons composed of coupled atomic chains on different substrates using the tight-binding Hamiltonian and Green’s function techniques. We have considered the spin-flip and spin-orbit couplings in the ribbon as well as electron leakage from chains to various types of substrates: with delocalized, weakly localized, and perfectly localized substrate electrons, which correspond to metallic, semiconductor, and insulator surfaces, respectively.

We have proposed coupled atomic chains with spin-dependent charge oscillations, where a ferromagnetic phase propagates only at both chain ends (for normal chains) or through the whole system (for topological chains). In particular, we have found strong asymmetry in the structure of the local DOS at atomic sites for short atomic systems due to (i) delocalized electrons in the substrate and (ii) due to spin-flip and spin-orbit couplings. In the former case, LDOS is spin-independent, and for perfectly localized electrons, the asymmetry in LDOS disappears. In the presence of the spin-flip and spin-orbit couplings, the structure of LDOS splits, moreover, is spin-dependent and LDOS asymmetry survives even for perfectly localized electrons in the substrate. These conclusions were verified for longer atomic systems in the presence of both spin-orbit couplings and the substrate electrons. As a main feature, we have found that for non-topological chains, only chain ends show spin-dependent LDOS characteristics, whereas the local DOS in the middle of the chain are spin-independent. As a result, such a chain reveals electron spin polarization only at its edges (ferromagnetic occupations), but in the middle of the chain, the occupations are the same for both spins (paramagnetic solutions). We have also investigated SSH spin-orbit chains and found spin-dependent Friedel oscillations along the whole chain. Note that in the SSH chain, without spin-flip and spin-orbit couplings, regular charge oscillations are not observed. The existence of spin-dependent oscillations of the occupations in the SSH chains is very important for potential applications of these structures in spin-memory devices. Additionally, we have found that the end topological states, which appear in the middle of the energy gap region, split in the presence of spin-flip and spin-orbit couplings and the appropriate local DOS structures are nonsymmetrical around the Fermi energy.

We have also found different periods of the local DOS oscillations (obtained for the Fermi energy at each atomic site) along the normal chain in the presence of spin-flip and spin-orbit couplings. These parameters renormalize the on-site electron energies in the system leading to the Friedel oscillations. The oscillations in coupled atomic chains (atomic ribbon) on a surface were investigated along the ribbon and we have found that minima and maxima of local DOS oscillations (between neighboring chains) are in phase for small spin-orbit parameters, but for larger couplings, these oscillations are out of phase. Of course, for larger spin-orbit couplings, strong asymmetry in the structure of the local DOS appears at both ribbon ends.

It is believed that our results can be verified experimentally using a spin-polarized STM tip for normal or SSH chains localized at different substrates which are the thinnest possible electric wires. Considered here atomic chains can be widely applied in nanoelectronics as their physical parameters can be precisely controlled using external fields or electrodes.

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