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Dopant ion concentrations in the sides of a symmetric quantum well are known to create a random Rashba-type spin-orbit coupling. Here, we demonstrate that, as a consequence, a finite size spin Hall effect is also present. Our numerical algorithm estimates the result of the Kubo formula for the spin Hall conductivity by using a tight-binding approximation of the Hamiltonian in the framework of a time-dependent Green's function formalism well suited for very large systems.

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When first discussed almost 50 years ago,[1] the Rashba-type spin-orbit (SO) coupling was attributed to the inversion asymmetry in zinc-blende quantum wells grown along the [001] direction. In this picture, the SO interaction is linear in the electron momentum $\mathbf{p}$ and is written in terms of the Pauli spin operators $\{\sigma_x, \sigma_y, \sigma_z\}$ as

$$H_{\mathrm{SO}} = \alpha(\sigma_x k_y - \sigma_y k_x). \tag{1}$$

The coupling constant α is a constant proportional to the gradient of the electric potential across the well and is thus tunable by an electric gate.[2]

Searching for ways and means of manipulating the electron spin in solid structures by electric fields, within the context of possible spintronics applications, has rekindled the interest in the Rashba model, and numerous studies[3,4] have been dedicated in the past several years to understanding all of the implications of this interaction on electron transport in reduced dimensionality semiconductor structures. Even though the original Rashba interaction is intrinsically linked to the quantum well asymmetry, a recent argument was made[5] for the existence of a random SO coupling that appears even in a perfectly symmetric quantum well on account of the changes in the dopant ion concentration on the sides of the well. This result is made possible by the existence of a local electric field, of random magnitude, perpendicular on the layer, at each point inside the well. Even though the spatial average of the random Rashba field that ensues is zero, it has been demonstrated that it puts a certain imprint on various electronic properties, such as the spin-relaxation rate that acquires a minimum value. Moreover, in the presence of a magnetic field, the effects of the random Rashba fields lead to longer spin-relaxation rates and a nonexponential spin relaxation.[6]

These ideas suggest the existence of a finite spin polarization that can be maintained also during spin transport. It is quite natural, therefore, to ask what happens to the spin Hall conductivity in this situation. The present work investigates the effect of the random Rashba field in symmetric quantum wells on the spin Hall conductivity, with the intention of appreciating its robustness against the natural variations of this type of SO coupling. Within a numerical algorithm based on the direct integration of the time-dependent modified Schrödinger equation, we establish that, indeed, a minimum spin Hall effect arises, which is dependent on the dopant ion concentration, that is quite resilient under the fluctuations of the random SO coupling.

The physical model of our system consists of a two-dimensional (2D) quantum well sandwiched between two doped layers of different concentrations, which are separated by a distance z_0. The dopant ions, which are assimilated with a δ-type perturbation, are assumed to have a charge e and are localized by a 2D in-plane vector $\mathbf{r}_i=(x_i, y_i)$. The total ion concentration in each layer is $n(\mathbf{r})=\Sigma_j \delta(\mathbf{r}-\mathbf{r}_j)$. In the simplest approximation, the Rashba coupling constant is proportional to the z component of the Coulomb electric field generated by the impurities as follows:

$$E_z(\mathbf{r}) = \frac{ez_0}{\epsilon}\sum_j \frac{1}{[(\mathbf{r}-\mathbf{r}_j)^2 + z_0^2]^{3/2}}, \tag{2}$$

where ϵ is the dielectric constant and the summation is performed over all the dopant sites in both layers. Hence, α depends both on position $\mathbf{r}$ and on the dopant distribution. In general, we can write that $\alpha_R(\mathbf{r})=\alpha_R e E_z(\mathbf{r})$, where α_R is some phenomenological system-dependent constant parameter. An illustration of this analysis is presented in Fig. 1, wherein values of $\alpha_R(\mathbf{r})$ are shown for two different impurity concentrations, for a system size of 400×400 nm and for $z_0=5$ nm.

Since the position-dependent SO coupling constant $\alpha_R(\mathbf{r})$ no longer commutes with the momentum operator, the single-particle Hamiltonian that describes the dynamics of an electron of momentum $\mathbf{p}$ and effective mass m^* acquires a symmetric form,

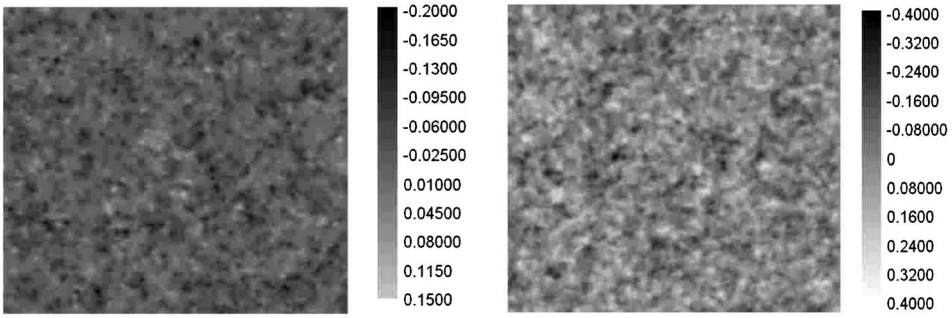

FIG. 1. Spatial dependence of the Rashba spin-orbit interaction for different values of n_u and n_d, which are the concentration of the carriers on the up and down sides of the well, respectively. Left: $n_u=10^{12}$ cm^{-2} and $n_d=5\times10^{11}$ cm^{-2}. Right: $n_{d,u}=5\times10^{12}$ cm^{-2}. In both figures, the system size is 400×400 nm and z_0 is fixed to 4 nm. The energetic units are relative to t_0, which is the hopping integral.

$$\tilde{H}=\frac{p^2}{2m^*}+\frac{1}{2}\{\alpha_R(r),\sigma_x p_y-\sigma_y p_x\}, \tag{3}$$

where $\{A,B\}$ represents the anticommutator of operators A and B. The Hamiltonian thus defined in Eq. (3) contains not just H_{SO}, which is the original Rashba Hamiltonian [Eq. (1)] written for $\alpha_R(\mathbf{r})$, but also an additional part, H_{random}, that reflects the noncommutativity of momentum and position operators involved explicitly in $\alpha_R(\mathbf{r})$,

$$\tilde{H}_{\mathrm{random}}=\frac{i}{2}\left[\sigma_y\frac{\partial\alpha_R(\mathbf{r})}{\partial x}-\sigma_x\frac{\partial\alpha_R(\mathbf{r})}{\partial y}\right]. \tag{4}$$

We note that $\tilde{H}_{\mathrm{random}}$ gives no contribution to other important characteristics of the system, such as the spin-dependent force operator $F_H\sim\alpha_R^2(\mathbf{r})$, which is entirely generated by H_{SO}.[7]

Inspired by Eq. (3), we directly write the Hamiltonian of the total system of electrons within the tight-binding approximation, generating an expression suitable for numerical calculations. Thus,

$$\begin{aligned}H=&\sum_{i,\alpha}\varepsilon_{i\alpha}c_{i\alpha}^{\dagger}c_{i\alpha}-\sum_{\langle i,j\rangle,\alpha}t_0c_{i\alpha}^{\dagger}c_{j\alpha}\\&+\sum_{i,\delta_x,\delta_y}V_R(i)[(c_{i\uparrow}^{\dagger}c_{i+\delta_x\downarrow}-c_{i\downarrow}^{\dagger}c_{i+\delta_x\uparrow})\\&-i\,(c_{i\uparrow}^{\dagger}c_{i+\delta_y\downarrow}+c_{i\downarrow}^{\dagger}c_{i+\delta_y\uparrow})].\end{aligned} \tag{5}$$

Here, $c_{i\alpha}^{\dagger}$ is the creation operator at site index i with spin α, and δ_x and δ_y are unit vectors along the x and y directions. An immediate consequence of the randomness of the Rashba spin-orbit strength is the site dependence of the parameters that describe the model. First, an on-site energy $\epsilon_{i\alpha}$ that depends on the gradient components of the electric field appears, which is similar to the case of disorder. The difference, however, is that in this case, the disorder is spatially correlated. Then, the Rashba coupling $V_R(i)=\alpha_R(i)/a_0$, which is written for a lattice constant a_0, depends on the values of the electric fields at neighbor sites. The hopping coupling t_0 has the usual expression $t_0=1/2m^*a_0^2$. In the following estimates, we fix its value at $t_0=12$ meV, which corresponds to a lattice constant $a_0\simeq2$ nm. (Throughout this work, $\hbar=1$, and free boundary conditions are used.) At the same time, the charge concentration fixes the Fermi energy ϵ_F through the relation $n=2m\epsilon_F/2\pi\hbar^2=10^{12}$ cm^{-2}. A numerical estimate of the spin Hall conductivity in a random environment, for large system sizes, can be obtained by using the Kubo formalism in the framework proposed by Tanaka and Itoh.[8] This method can be, in principle, used for the calculation of any expectation value of any combinations of Green's functions and quantum operators, such as the density of states, or conductivity.[8,9] Besides, it is well suited for large systems wherein traditional methods such as direct diagonalization fails due to memory problems. Within this algorithm, for a given field distribution, the on-site energies, hopping probabilities, and the Rashba field are computed first at each site. Then, the spin-Hall conductivity is calculated for a given configuration.

The main steps involved in performing the numerical calculations are outlined below. The computation starts from solving the time-dependent modified Schrödinger equation, with a single-frequency source term,

$$i\frac{d|\tilde{j},t\rangle}{dt}=H|\tilde{j},t\rangle+|j\rangle\theta(t)\exp^{-i(E+i\eta)t}, \tag{6}$$

where η is a finite small value and θ is the step function.

To determine the time evolution of the state ket $|\tilde{j};t\rangle$, a direct numerical integration of the modified Schrödinger equation is performed, using the "leap-frog" algorithm.[10] This is a second order symmetrized differencing scheme, which is accurate up to $(H\Delta t)^2$. In this approximation, Eq. (6) becomes

$$|\tilde{j};t+\Delta t\rangle=-2i\Delta tH|\tilde{j};t\rangle+|\tilde{j};t-\Delta t\rangle-2i\Delta t|j\rangle e^{-i(E+i\eta)t}\theta(t). \tag{7}$$

The time step Δt is determined by $\Delta t\simeq\beta/|E|$, where $|E|$ is the absolute value of the energy and β is a parameter whose value is less than 1 in order for the solution to be stable.

An analytic solution of Eq. (6) with the initial condition $|\tilde{j},t=0\rangle=0$ is written as

$$|\tilde{j},t\rangle = -i\int_0^t dt' e^{-iH(t-t')}|j\rangle e^{-i(E+i\eta)t'}$$

$$= \frac{1}{E+i\eta-H}[e^{-i(E+i\eta)t} - e^{-iHt}]|j\rangle, \quad (8)$$

where one recognizes the Green's function operator $(E+i\eta-H)^{-1}$ as the prefactor in the final expression. For a sufficiently large time, the Green's function operating on the ket $|j\rangle$ can be obtained with a relative accuracy $\delta=e^{-\eta T}$ by inverting Eq. (8) as

$$G(E+i\eta)|j\rangle = \lim_{T\to\infty}|\tilde{j},T\rangle e^{i(E+i\eta)T}. \quad (9)$$

Consequently, the matrix element between any two states $\langle i|$ and $|j\rangle$ is obtained as

$$\langle i|G(E+i\eta)|j\rangle = \lim_{T\to\infty}\langle i|\tilde{j},T\rangle. \quad (10)$$

These results can be easily generalized to the case when a product including several Green's functions and operators is involved by choosing a new initial state, such as $|j'\rangle = AG(E+i\eta)|j\rangle$ in Eq. (6), and repeating the same procedure. In a similar fashion, the method can be generalized to the case when many different energy values are considered. In this case, one simultaneously solves Eq. (6) for a source term with multiple frequencies, $|j\rangle(\Sigma_l e^{-i(E_l+i\eta)t})\theta(t)$.

The efficiency of the algorithm is increased if, instead of a local orbital basis set, a randomized version of this basis is selected. This can be described by a ket, $|\phi\rangle=\Sigma_{n=1}^{N}|n\rangle\exp(-i\phi_n)$, where $|n\rangle$ are the localized orbitals and ϕ_n are random numbers in the $[0,2\pi]$ interval. Then, the average of a given operator A is calculated as

$$\langle\phi|A|\phi\rangle \simeq \sum_n \langle n|A|n\rangle + O\left(\frac{1}{\sqrt{N}}\right), \quad (11)$$

within the statistical errors of $1/\sqrt{N}$. It was shown[11] that this choice of basis is the best one for reducing the numerical errors.

As a first application of the present method, we calculate the density of states,

$$\varrho(\omega) = -\frac{1}{\pi}\mathrm{Im}[\mathrm{Tr}\ G(\omega+i\eta)], \quad (12)$$

in a system size of $200a_0\times 200a_0$ for a constant V_R. The results, which are computed for three different values of V_R, are presented in Fig. 2.

In the presence of a constant Rashba field, the band structure suffers two important modifications. First, the bandwidth proportionally increases with V_R as a consequence of the renormalization of the hopping probability by the Rashba interaction. Second, the Van Hove singularity in the density of states that occurs at zero energy when $V_R=0$ splits when V_R is turned on. This corresponds to the splitting and shifting of the original spin-degenerate band into the two chiral subbands, characteristic to the Rashba model. Analytically, it

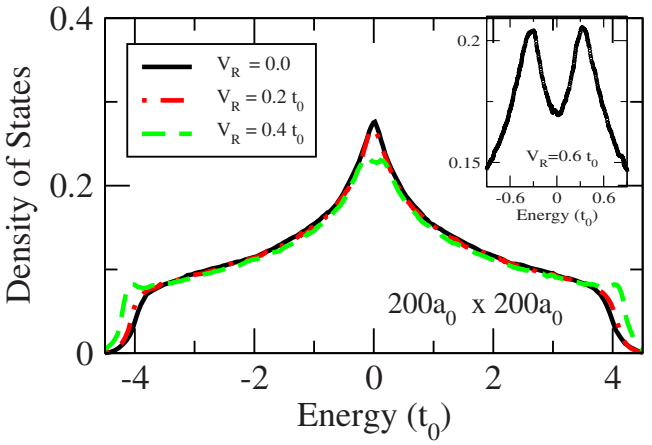

FIG. 2. (Color online) The density of states of a clean system with constant Rashba coupling V_R is calculated for a square lattice with a size of $200\times 200a_0$. The energy is expressed in hopping-integral units, t_0.

can be shown[12] that the splitting is proportional with V_R^2. This behavior can be observed in the inset of Fig. 2 wherein a large $V_R=0.6t_0$ was considered.

The spin Hall conductivity can be calculated with the Kubo formula,

$$\sigma_{sH} = \frac{1}{2}\mathrm{Tr}\int\frac{d\varepsilon}{2\pi}\left[-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right]\langle j_x^z[G_R(\varepsilon)-G_A(\varepsilon)]v_y G_A(\varepsilon)$$

$$- j_x^z G_R(\varepsilon)v_y[G_R(\varepsilon)-G_A(\varepsilon)]\rangle. \quad (13)$$

This expression considers contributions only from states at the Fermi surface, as indicated by the presence of the sharply peaked derivative of the distribution function. Such an approximation is justified by previous studies of the spin Hall effect, which demonstrated that states below the Fermi surface does not contribute to the spin Hall conductivity and that spin Hall conductivity entirely comes from quasiparticle states at the Fermi level.[13]

In Eq. (13), the velocity operator is defined by the commutator $iv_y=[y,H]$, whereas the spin current along the $\hat{x}$ direction given in terms of the anticommutator between the velocity operator and the Pauli matrix σ_z, $j_x^z=\{\sigma_z,v_x\}/4$.[14] $G_{R/A}(\epsilon)$ represents the retarded and/or advanced Green's function.

For a constant Rashba field, the algorithm outlined above generates results, which after being averaged over 200 different impurity distributions are presented in Fig. 3.

For any value of V_R, the universally predicted value of $\sigma_{sH}=e/8\pi$ is reached, but only for some energy interval inside the band. Usually, the spin Hall conductivity is smaller than $e/8\pi$. It decreases as the band edges are approached and vanishes beyond them. This behavior is preserved for system sizes of up to $500a_0\times 500a_0$, indicating that the system remains in the ballistic regime regardless of its size for as long as no disorder is included. In the right inset of Fig. 3, we present the η dependence of the spin Hall conductivity. For values smaller than 0.1, already the convergence to the appropriate value is reached. Increasing η above 0.1 deviations is already consistent even if a larger integration time is

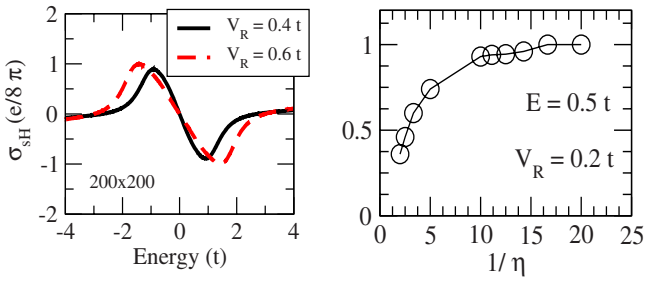

FIG. 3. (Color online) Left: The spin Hall conductivity for a clean system with a size of $200\times200a_0$, with a constant V_R. The results are obtained by averaging over 200 initial wave functions. Right: η dependence of the spin Hall conductance for a fixed energy $E=0.5t$ and a Rashba coupling $V_R=0.2t$. The error bars are smaller than the size of the symbols.

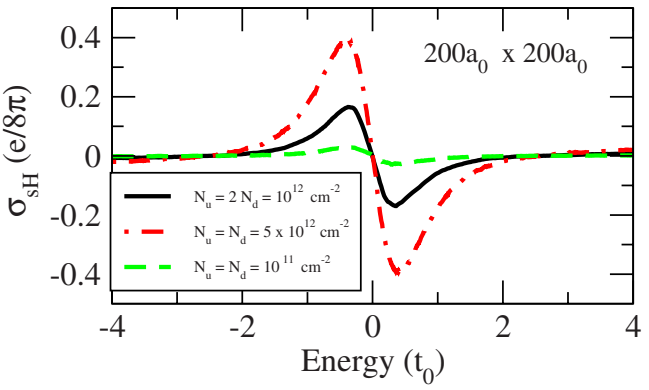

FIG. 4. (Color online) The spin Hall conductivity when both up-down doping layers are present. For each Rashba field distribution, the spin-Hall conductivity was averaged over 200 initial wave functions at each energy. The figure presents averages over 100 random impurity configurations.

used. Throughout of our calculations, we have used $\eta=0.1$. Similar results for the spin Hall conductance were obtained by using a Landauer–Büttiker formalism.[7]

Calculated values of the spin Hall conductivity in the presence of a random Rashba field, averaged over 100 impurity configurations, are shown in Fig. 4 for different dopant concentrations of the sides of the well, u (up) and d (down), respectively.

Here, the randomness of the electric field created by the dopants generate a Rashba coupling at each lattice site, even in the absence of an external Rashba field. A finite σ_{sH} is still obtained. The parameters used for our analysis are experimentally reachable.[2] The solid and dashed-dotted lines in Fig. 4 correspond to the spatial distribution of the Rashba fields presented in Fig. 1.

When a symmetric distribution of the impurity ions is considered on the sides of the well, a vanishingly small Rashba field ensues when averaged over the entire sample, as shown in Fig. 1. The corresponding spin Hall conductivity, however, which is determined by the configuration average of the spatial variation of the coupling constant α, increases as expected with the impurity concentration and seems to be favored by perfectly symmetric distributions. When the numbers of impurities are different on the sides of the quantum well, the average Rashba field is finite, but the spin Hall conductivity decreases. A possible explanation of this result can be given in terms of the spatial correlation of the spin-orbit interaction over the spin precession length[5] that is strong enough to assure the existence of a finite spin Hall effect even in the case of a null average spin-orbit field.

In conclusion, we have studied the spin-Hall effect in a perfectly symmetric quantum well when fluctuations of the Rashba spin-orbit interaction field are considered as arising due to the impurities on the sides of the well. Even in the extreme limit, when an equal number of the impurities generate a Rashba field averaged to a very small value, a finite spin Hall conductivity seems to exist in the system in the range of 5%–10% of the original universal value $e/8\pi$.

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