Limitation of electron mobility from hyperfine interaction in ultraclean quantum wells and topological insulators

S. A. Tarasenko*
Ioffe Institute, 194021 St. Petersburg, Russia

Guido Burkard
Department of Physics, University of Konstanz, D-78464 Konstanz, Germany
(Received 31 August 2015; revised manuscript received 4 May 2016; published 19 July 2016)

The study of electron transport and scattering processes limiting electron mobility in high-quality semiconductor structures is central to solid-state electronics. Here, we uncover an unavoidable source of electron scattering which is caused by fluctuations of nuclear spins. We calculate the momentum relaxation time of electrons in quantum wells governed by the hyperfine interaction between electrons and nuclei and show that this time depends greatly on the spatial correlation of nuclear spins. Moreover, the scattering processes accompanied by a spin flip are a source of the backscattering of Dirac fermions at conducting surfaces of topological insulators.

DOI: 10.1103/PhysRevB.94.045309

I. INTRODUCTION

The invention of modulation-doped semiconductor structures [1] and the subsequent progress in semiconductor technology have led to the fabrication of ultrahigh-mobility two-dimensional (2D) electron systems [2,3] and the discovery of novel exciting quantum phenomena such as the fractional quantum Hall effect [4] and microwave-induced resistance oscillations [5]. Much effort is focused now on the search for new technological approaches and the optimization of quantum well (QW) design to reduce structure disorder and increase electron mobility. This raises the question of the fundamental limitation of electron mobility that can be achieved in defect-free QW structures with ideal interfaces (see Ref. [6] for a recent discussion).

Here, we analyze a source of electron scattering stemming from hyperfine interaction between electron spins and spins of nuclei constituting the crystal lattice. This scattering mechanism is unavoidable in III–V compounds since all stable and long-lived isotopes of anions (N, P, As, Sb) and cations (B, Al, Ga, In) possess nonzero nuclear spins. The hyperfine interaction in semiconductors has been extensively studied in the context of coupled electron and nuclear spin dynamics in bulk semiconductors [7], in quantum dots (QDs) [8,9] and QWs [10–13], and also in spin-dependent electron transport along the edge channels of a 2D electron gas [14–19] or through QDs (spin-blockade effect) [20–23] but not in bulk charge transport measurements. Here, we calculate the electron mobility limited by electron-nuclear hyperfine interaction in QWs for various spin configurations of the electron and nuclear subsystems including the case of unpolarized electrons and nuclei and dynamic nuclear polarization (DNP). It is shown that the effect of electron-nuclear interaction on the electron mobility depends greatly on the spatial correlation of nuclear spins. Generally, both spin-conserving and spin-flip processes contribute to electron scattering. Quadrupole splitting of the nuclear spin levels in strained QWs or Zeeman splitting of the electron and nuclear levels in a magnetic field can suppress spin-flip electron scattering by nuclear spin fluctuations at low temperatures. A uniform nuclear polarization, achieved, e.g., by DNP, in turn suppresses the spin-conserving scattering processes. Spin-flip scattering is an unavoidable source of backscattering of 2D Dirac fermions emerging at conducting surfaces of topological insulators.

II. SCATTERING BY UNCORRELATED NUCLEAR SPINS

The effective Hamiltonian of hyperfine interaction between conduction-band electrons and nuclei can be presented in the form [7]

$$V = \sum_{\alpha,n} A_\alpha v_0 \, \boldsymbol{S} \cdot \boldsymbol{I}_{\alpha,n} \, \delta(\boldsymbol{r} - \boldsymbol{R}_{\alpha,n}), \tag{1}$$

where α is the index of nucleus species, n enumerates nuclei of certain species, A_α are the constants of interaction, v_0 is the volume of the primitive cell, $\boldsymbol{S}$ and $\boldsymbol{I}_{\alpha,n}$ are the electron and nucleus spin operators, respectively, and $\boldsymbol{R}_{\alpha,n} = (\boldsymbol{\rho}_{\alpha,n}, z_{\alpha,n})$ are the positions of the nuclei [24].

We assume first that nuclei are unpolarized on average and their spin states are uncorrelated with each other. Then, the scattering of an electron by different nuclei occurs independently and the total probability of the scattering from the initial state $(\boldsymbol{k},s)$ to the final state $(\boldsymbol{k}',s')$ is given by the golden rule rate,

$$W_{\boldsymbol{k}'s',\boldsymbol{k}s} = \frac{2\pi}{\hbar} \sum_{\alpha,n} \sum_{j,j'} \left| M^{(\alpha,n)}_{s'j',sj} \right|^2 p_{\alpha j} \times \delta(\varepsilon_k + \varepsilon_s + \varepsilon_{\alpha j} - \varepsilon_{k'} - \varepsilon_{s'} - \varepsilon_{\alpha j'}), \tag{2}$$

where $\boldsymbol{k}$ and $\boldsymbol{k}'$ are the wave vectors in the QW plane, $s,s' = \pm 1/2$ are the electron spin projections, j and j' are the initial and final nuclear spin projections, $M^{(\alpha,n)}_{s'j',sj}$ is the matrix element of scattering at the potential given in Eq. (1), $p_{\alpha j}$ is the nuclear spin distribution function, $\varepsilon_k = \hbar^2 k^2/(2m^*)$ is the electron kinetic energy, m^* is the effective mass, ε_s is the energy related to electron spin, e.g., in an external magnetic field, and $\varepsilon_{\alpha j}$ are the nuclear energies. The hyperfine interaction is weak and short-range compared to the de Broglie

*tarasenko@coherent.ioffe.ru

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wavelength of electrons. It allows us to study scattering in the first Born approximation and neglect screening.

The squared modulus of the scattering matrix element has the form

$$\left|M^{(\alpha,n)}_{s'j',sj}\right|^2 = A_\alpha^2 v_0^2 \left|\langle s'j'|\boldsymbol{S}\cdot\boldsymbol{I}_{\alpha,n}|sj\rangle\right|^2 \psi^4(z_{\alpha,n}), \quad (3)$$

where $\psi(z)$ is the function of electron size quantization in the QW. The operator $\boldsymbol{S}\cdot\boldsymbol{I}$ can be rewritten in the form

$$\boldsymbol{S}\cdot\boldsymbol{I} = S_z I_z + (S_+ I_- + S_- I_+)/2, \quad (4)$$

where $S_\pm = S_x \pm \mathrm{i}S_y$, $I_\pm = I_x \pm \mathrm{i}I_y$, and S_β and I_β ($\beta = x,y,z$) are the Cartesian components, which yields

$$\begin{aligned}&\langle s'j'|\boldsymbol{S}\cdot\boldsymbol{I}|sj\rangle\\ &= s\,j\,\delta_{s's}\delta_{j'j} + \tfrac{1}{2}\sqrt{(I-j)(I+j+1)}\,\delta_{s',s-1}\delta_{j',j+1}\\ &\quad + \tfrac{1}{2}\sqrt{(I-j+1)(I+j)}\,\delta_{s',s+1}\delta_{j',j-1}\,. \end{aligned} \quad (5)$$

The electron relaxation time τ_p determining the mobility is expressed via the probability of scattering, (2). To derive the expression for τ_p we follow Boltzmann's approach and write the collision integral, which plays the role of the "friction force" in Boltzmann's equation,

$$\mathrm{St} f_{\boldsymbol{k}s} = \sum_{\boldsymbol{k}'s'}[f_{\boldsymbol{k}'s'}(1-f_{\boldsymbol{k}s})W_{\boldsymbol{k}s,\boldsymbol{k}'s'} - f_{\boldsymbol{k}s}(1-f_{\boldsymbol{k}'s'})W_{\boldsymbol{k}'s',\boldsymbol{k}s}], \quad (6)$$

where $f_{\boldsymbol{k}s}$ is the electron distribution function. In the presence of a weak driving electric field, the distribution function has the form $f_{\boldsymbol{k}s} = f_s^{(0)}(\varepsilon_k) + \delta f_{\boldsymbol{k}s}$, where $f_s^{(0)}$ is the equilibrium function and $\delta f_{\boldsymbol{k}s}$ is a small anisotropic correction. To first order in $\delta f_{\boldsymbol{k}s}$ and for $W_{\boldsymbol{k}s,\boldsymbol{k}'s'}$ independent of the directions of the wave vectors $\boldsymbol{k}$ and $\boldsymbol{k}'$, which is valid for short-range scattering by nuclei, Eq. (6) yields

$$\mathrm{St} f_{\boldsymbol{k}s} = -\frac{\delta f_{\boldsymbol{k}s}}{\tau_p}, \quad (7)$$

where

$$\tau_p^{-1} = \sum_{\boldsymbol{k}'s'}\left\{f_{s'}^{(0)}(\varepsilon_{k'})W_{\boldsymbol{k}s,\boldsymbol{k}'s'} + \left[1-f_{s'}^{(0)}(\varepsilon_{k'})\right]W_{\boldsymbol{k}'s',\boldsymbol{k}s}\right\}. \quad (8)$$

Finally, for the scattering probability given by Eq. (2), homogeneously distributed nuclei and degenerate electron gas, we obtain

$$\begin{aligned}\tau_p^{-1} &= \frac{m^*}{\hbar^3}\int \psi^4(z)dz \sum_\alpha A_\alpha^2 v_0^2 N_\alpha \sum_{jj's'} |\langle s'j'|\boldsymbol{S}\cdot\boldsymbol{I}_\alpha|sj\rangle|^2\\ &\quad\times\left[p_{\alpha j} + (p_{\alpha j'} - p_{\alpha j})f_{s'}^{(0)}(E_F + \varepsilon_{\alpha j} - \varepsilon_{s'} - \varepsilon_{\alpha j'})\right]\\ &\quad\times\theta(E_F + \varepsilon_{\alpha j} - \varepsilon_{s'} - \varepsilon_{\alpha j'}), \end{aligned} \quad (9)$$

where N_α are the densities of nuclei of certain species, E_F is the Fermi energy, and $\theta(\varepsilon)$ is the Heaviside step function. We note that, for rectangular QWs with infinitely high barriers, $\int \psi^4(z)dz = 3/(2d)$, with d being the QW width. Also note that, in general, τ_p can depend on the electron spin s unless the nuclear-spin distribution is symmetric, $p_j = p_{-j}$. The time-reversal symmetry imposing the condition $p_j = p_{-j}$ can be broken by an external magnetic field or DNP (studied below), spontaneously (see discussions of the possibility of nuclear self-polarization in Refs. [7] and [25]), or, in principle, by the driving of an electric current through the quantum well. In the latter case, the electric current induces a spin polarization of electrons due to spin-orbit coupling, which results, in turn, in a buildup of DNP [26]. The emerging electron and nuclear spin polarizations are both proportional to the electric current and, therefore, do not affect the linear electron transport. Nonlinear effects are beyond the scope of this paper. Below, we analyze Eq. (9) for some particular cases which are of interest.

(i) All spin states of nuclei are degenerate and equally populated, $\varepsilon_{\alpha j} = 0$, $p_{\alpha j} = 1/(2I_\alpha + 1)$, where I_α are the nuclear spins; electrons are unpolarized, $\varepsilon_s = 0$. In this case, both spin-conserving and spin-flip scattering processes are allowed. Taking into account that

$$\sum_j |\langle s\,j|\boldsymbol{S}\cdot\boldsymbol{I}|s\,j\rangle|^2 = I(I+1)(2I+1)/12,$$

$$\sum_j |\langle s\pm 1, j\mp 1|\boldsymbol{S}\cdot\boldsymbol{I}|s,j\rangle|^2 = I(I+1)(2I+1)/6,$$

we obtain

$$\tau_p^{-1} = \frac{m^*}{4\hbar^3}\int \psi^4(z)dz \sum_\alpha A_\alpha^2 v_0^2 N_\alpha I_\alpha(I_\alpha+1). \quad (10)$$

We note that spin-flip scattering processes in the context of electron and nuclear spin relaxation were theoretically considered in Ref. [12].

The degeneracy of nuclear spin levels may be lifted due to the quadrupole interaction of nuclear spins with the strain-induced gradient of the crystal field in lattice-mismatched structures [8]. In a simple axial model relevant for (001)-oriented QWs, the quadrupole interaction determining the splitting and order of the spin levels is proportional to I_z^2, i.e., levels with different j^2 values have different energies. The sign of the quadrupole splitting is opposite for axial tension and compression. Typical values of the quadrupole splitting in III–V heterostructures are of the order of 1–10 neV, which corresponds to 10^{-5}–10^{-4} K on the temperature scale [8,27]. Therefore, nonequal thermal populations of the nuclear spin levels at submillikelvin (sub-mK) temperatures can occur and affect the electron-nuclear interaction.

(ii) Nuclear spin levels are split by strain in such a way that the ground levels are characterized by the highest spin projections, $j = \pm I_\alpha$, $I_\alpha > 1/2$; electrons are unpolarized, $\varepsilon_s = 0$. The temperature is lower than the nuclear quadrupole splitting, and therefore, only ground levels contribute to scattering; $p_{\alpha j} = 1/2$ if $j = \pm I_\alpha$ and $p_{\alpha j} = 0$ otherwise. Only spin-conserving scattering processes can occur and the corresponding electron relaxation time is given by

$$\tau_p^{-1} = \frac{m^*}{4\hbar^3}\int \psi^4(z)dz \sum_\alpha A_\alpha^2 v_0^2 N_\alpha I_\alpha^2. \quad (11)$$

(iii) Nuclear spin levels are split by strain in such a way that the ground levels are characterized by the lowest spin projections $j = \pm 1/2$, and I_α is a half-integer; electrons are unpolarized, $\varepsilon_s = 0$. The temperature is lower than the quadrupole splitting energy and only ground levels contribute

to scattering, $p_{\alpha,\pm 1/2} = 1/2$. In this case, both spin-flip and spin-conserving processes contribute to scattering and the electron relaxation time has the form

$$\tau_p^{-1} = \frac{m^*}{8\hbar^3}\int \psi^4(z)dz \sum_\alpha A_\alpha^2 v_0^2 N_\alpha [1/2 + (I_\alpha + 1/2)^2]. \tag{12}$$

(iv) All spin states of nuclei are degenerate and equally populated, $\varepsilon_{\alpha j} = 0$, $p_{\alpha j} = 1/(2I_\alpha + 1)$; electrons are completely spin polarized by an external magnetic field (thermal nuclear polarization is small and neglected). In this particular case, only spin-conserving processes can occur and Eq. (9) yields

$$\tau_p^{-1} = \frac{m^*}{12\hbar^3}\int \psi^4(z)dz \sum_\alpha A_\alpha^2 v_0^2 N_\alpha I_\alpha(I_\alpha + 1). \tag{13}$$

In III–V semiconductor structures, nuclear spins can be efficiently polarized by DNP [7,8]. In the case of uniform nuclear polarization, the average nuclear field should be excluded from the Hamiltonian of the electron-nuclear interaction causing electron scattering because it does not introduce any disorder which breaks the translational symmetry of the crystal lattice. Accordingly, the operators $\boldsymbol{I}_\alpha$ in Eqs. (3) and (9) should be replaced with $\boldsymbol{I}_\alpha - \tilde{\boldsymbol{I}}_\alpha$, where the vectors $\tilde{\boldsymbol{I}}_\alpha$ are given by

$$\tilde{\boldsymbol{I}}_\alpha = \frac{\sum_\beta A_\beta N_\beta \bar{\boldsymbol{I}}_\beta}{A_\alpha \sum_\beta N_\beta}; \tag{14}$$

the index β runs over the nuclei of anions or cations if α stands for the nucleus of an anion or a cation, respectively, and $\bar{\boldsymbol{I}}_\alpha$ is the average nuclear spin of a certain isotope. In the simple case of an isotopically pure crystal, where all anions and cations are of certain isotopes, $\tilde{\boldsymbol{I}}_\alpha = \bar{\boldsymbol{I}}_\alpha$. We assume that all the vectors $\bar{\boldsymbol{I}}_\alpha$ point along the same axis z and choose z as the spin quantization axis. Then one obtains $\bar{I}_\alpha = \bar{j}_\alpha = \sum_j j p_{\alpha j}$ and the scattering marix elements

$$\begin{aligned}\langle s'j'|\boldsymbol{S}\cdot(\boldsymbol{I}_\alpha - \tilde{\boldsymbol{I}}_\alpha)|sj\rangle &= s\,(j - \tilde{I}_\alpha)\,\delta_{s's}\delta_{j'j} \\ &\quad + \tfrac{1}{2}\sqrt{(I_\alpha - j)(I_\alpha + j + 1)}\,\delta_{s',s-1}\delta_{j',j+1} \\ &\quad + \tfrac{1}{2}\sqrt{(I_\alpha - j + 1)(I_\alpha + j)}\,\delta_{s',s+1}\delta_{j',j-1}.\end{aligned} \tag{15}$$

Now we discuss the electron relaxation time in the presence of DNP.

(v) Nuclei are spin polarized; electrons of both spin states are present at the Fermi level. The splitting of nuclear levels is lower than the temperature so that both spin-conserving and spin-flip processes can contribute to scattering. Under such conditions, the momentum relaxation time becomes spin dependent and is given by

$$\begin{aligned}\tau_{p,s}^{-1} = \frac{m^*}{4\hbar^3}\int \psi^4(z)dz \sum_\alpha A_\alpha^2 v_0^2 N_\alpha \big[I_\alpha^2 \\ + I_\alpha + \tilde{I}_\alpha^2 - 2\bar{j}_\alpha(\tilde{I}_\alpha + s)\big].\end{aligned} \tag{16}$$

(vi) Nuclei are spin polarized; electrons are completely spin polarized by the nuclear (Overhauser) effective magnetic field or an external magnetic field. Then, only spin-conserving scattering occurs and we obtain the relaxation time

$$\tau_p^{-1} = \frac{m^*}{4\hbar^3}\int \psi^4(z)dz \sum_\alpha A_\alpha^2 v_0^2 N_\alpha \big[\overline{j_\alpha^2} - 2\bar{j}_\alpha \tilde{I}_\alpha + \tilde{I}_\alpha^2\big], \tag{17}$$

where $\overline{j_\alpha^2} = \sum_j j^2 p_{\alpha j}$. For isotopically purified crystals, the expression in brackets is reduced to $\overline{j_\alpha^2} - \bar{j}_\alpha^2$. This quantity is 0 for fully polarized nuclei when both $\overline{j_\alpha^2}$ and $\bar{j}_\alpha^2$ are equal to I_α^2. The absence of spin-conserving electron scattering by fully polarized nuclei, when crystal translational symmetry is restored, is in accordance with the free motion of Bloch electrons in a periodic potential. In isotopically mixed QW structures, scattering may occur even in the case of fully polarized nuclei due to the disorder caused by a difference in the nuclear spins I_α and/or the interaction constants A_α of anions (or cations). The corresponding relaxation time is given by

$$\tau_p^{-1} = \frac{m^*}{4\hbar^3}\int \psi^4(z)dz \sum_\alpha A_\alpha^2 v_0^2 N_\alpha (I_\alpha - \tilde{I}_\alpha)^2. \tag{18}$$

Now we estimate the electron relaxation time governed by the scattering from unpolarized nuclei following Eq. (10). The estimation for a 10-nm-wide QW grown from GaAs, where $m^* \approx 0.067 m_0$, with m_0 being the free electron mass, $I_{\mathrm{Ga}} = 3/2$, $I_{\mathrm{As}} = 3/2$, and $v_0^2 \sum_\alpha A_\alpha^2 N_\alpha \approx 0.2 \times 10^{-24}$ meV^2 cm^3 [28], is $\tau_p \sim 10^{-5}$ s. This corresponds to a mobility $\mu \sim 4 \times 10^{11}$ cm^2/(V s), which is still a few orders of magnitude higher than the mobility achieved to date [2]. The relaxation time governed by the hyperfine interaction can be much shorter in structures made of atoms with large nuclear spins (e.g., $I_{\mathrm{In}} = 9/2$) or heavy atoms, where the interaction constants are larger.

The probabilities of spin-conserving and spin-flip processes are comparable. Therefore, electron scattering by unpolarized nuclei makes a contribution to electron spin relaxation with the time τ_s comparable to the momentum relaxation time τ_p calculated above. This spin relaxation mechanism can be important if other mechanisms are suppressed, e.g., in (110)-oriented QWs, where the D'yakonov-Perel' spin relaxation mechanism is suppressed for the out-of-plane spin component [29–31] and a spin lifetime of up to 0.5 μs was recently determined [32].

III. SCATTERING OF DIRAC FERMIONS

Spin-flip processes contribute to the backscattering of 2D Dirac fermions emerging at surfaces of 3D topological insulators. In such materials, the strong spin-orbit interaction giving rise to topologically protected surface states locks the carrier spin and momentum [33]. Therefore, elastic scattering between states with opposite momenta is forbidden in the presence of time-reversal symmetry. Interaction with nuclear spins breaks the time-reversal symmetry in the subsystem of the Dirac fermions and enables backscattering. Electron-nuclear interaction leading to backscattering between 1D helical edge states of 2D topological insulators was studied in Refs. [18] and [19]. Here, we calculate the probability of scattering for 2D Dirac fermions on surfaces of 3D topological insulators and provide estimates for HgTe and Bi_2Se_3.

HgTe is a gapless semiconductor with an inverted band structure which becomes a 3D topological insulator if strained and the strain opens a gap in the otherwise fourfold degenerate Γ_8 states [34,35]. Within the six-band $\boldsymbol{k}\cdot\boldsymbol{p}$ theory, relevant for narrow-band materials, the topological surface states are described by the wave functions

$$\Psi_{\boldsymbol{k}}(\boldsymbol{\rho},z) = \left[\sum_{m=\pm1/2}\psi_{\Gamma_6,m}(z)|\Gamma_6,m\rangle + \sum_{m=\pm1/2,\pm3/2}\psi_{\Gamma_8,m}(z)|\Gamma_8,m\rangle\right]\exp(i\boldsymbol{k}\cdot\boldsymbol{\rho}), \tag{19}$$

where $\psi_{\Gamma_6,m}(z)$ and $\psi_{\Gamma_8,m}(z)$ are the envelope functions in the direction normal to the surface, $|\Gamma_6,m\rangle$ and $|\Gamma_8,m\rangle$ are the basis Bloch amplitudes of the s-type Γ_6 and p-type Γ_8 states, respectively, and $\boldsymbol{k}$ is the wave vector in the surface plane. For strained HgTe films, the wave function, (19), contains a considerable contribution ($\sim$20%) from the Γ_6 states [35]. Since the hyperfine interaction for s-type Bloch amplitudes given by the Fermi contact term is much stronger than that for p-type Bloch amplitudes [8,36], a good estimation is that the electron-nuclear interaction for Dirac fermions at the HgTe surface is of contact type and determined by the contribution of the Γ_6 states.

The electron spin of surface states in the axial approximation lies in the surface plane and points perpendicular to the wave vector. Accordingly, a spinor composed of the functions $\psi_{\Gamma_6,\pm1/2}(z)$ can be presented in the form

$$\begin{bmatrix}\psi_{\Gamma_6,+1/2}(z)\\ \psi_{\Gamma_6,-1/2}(z)\end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\ i\exp(i\varphi_{\boldsymbol{k}})\end{bmatrix}\psi_{\Gamma_6}(z), \tag{20}$$

where $\varphi_{\boldsymbol{k}}$ is the polar angle of the vector $\boldsymbol{k}$. Following Eqs. (1) and (5) one can readily calculate the matrix element of scattering. For scattering from the initial state $\boldsymbol{k}$ to the final state $\boldsymbol{k}'$ the squared modulus of the scattering matrix element has the form

$$\left|M^{(\alpha,n)}_{\boldsymbol{k}'j',\boldsymbol{k}j}\right|^2 = \tfrac{1}{16}A_\alpha^2 v_0^2\,|\psi_{\Gamma_6}(z_{\alpha,n})|^4[4\sin^2(\theta/2)\,j^2\delta_{j'j} + (I_\alpha - j+1)(I_\alpha+j)\delta_{j',j-1} + (I_\alpha - j)(I_\alpha+j+1)\delta_{j',j+1}],$$

where $\theta = \varphi_{\boldsymbol{k}'} - \varphi_{\boldsymbol{k}}$ is the angle of scattering.

The differential probability of elastic scattering of a test particle by the angle θ in 2D systems is given by

$$dw(\theta) = \frac{k}{2\pi\hbar^2 v}\sum_{\alpha,n}\sum_{j,j'}\left|M^{(\alpha,n)}_{\boldsymbol{k}'j',\boldsymbol{k}j}\right|^2 p_{\alpha j}\,d\theta, \tag{21}$$

where $v = (1/\hbar)d\varepsilon_k/dk$ is the velocity, which is independent of the energy for linearly dispersive Dirac fermions.

We assume that all spin states of the nuclei are degenerate and equally populated, $p_{\alpha j} = 1/(2I_\alpha+1)$. Then, summing up over the nuclei, we obtain

$$dw(\theta) = \frac{k}{24\pi\hbar^2 v}[1+\sin^2(\theta/2)]d\theta \times \int\left|\psi_{\Gamma_6}(z)\right|^4 dz\sum_\alpha A_\alpha^2 v_0^2 N_\alpha\, I_\alpha(I_\alpha+1). \tag{22}$$

Equation (22) describes the scattering of 2D Dirac fermions by nuclear spin fluctuations. It shows that the backscattering ($\theta = \pi$) determined by spin-flip processes is twice as efficient as the forward scattering ($\theta = 0$) determined by spin-conserving processes.

In natural HgTe, about 30% of Hg nuclei and about 8% of Te nuclei possess nonzero spins [19]. To the best of our knowledge, the hyperfine interaction constants have not been measured yet. Considering the fraction of nuclei with nonzero spins, the typical parameters of surface states in HgTe films [35] ($k = 2\times10^6$ cm^{-1}, $v = 0.5\times10^8$ cm/s, characteristic length of surface-state localization $d = 10$ nm, and Γ_6 band partition of 0.2), we estimate that the probability of scattering by nuclear spin fluctuations is two to three orders of magnitude lower than that in GaAs quantum wells.

Other prominent examples of 3D TIs are binary and ternary compounds of Bi with Se and Te [33]. Natural Bi consists of the only isotope ^{209}Bi with nuclear spin 9/2. Recent measurements of nuclear magnetic resonance in n-type Bi_2Se_3 crystals have revealed very strong contact interactions between electrons and ^{209}Bi nuclei (in spite of the fact that the Bloch amplitude is mostly of the p type) [37]. The contact hyperfine interaction constant is found to be comparable to and even exceed those for conduction-band electrons in GaAs. These results suggest that the scattering of Dirac fermions at the Bi_2Se_3 surface by nuclear spin fluctuations can be as efficient as that of electrons in GaAs-based structures.

IV. SCATTERING BY FLUCTUATIONS OF MACROSCOPIC NUCLEAR POLARIZATION

The electron-nuclear interaction is drastically enhanced if the nuclear spins are spatially correlated and polarized at a macroscopic scale. Such a nuclear spin polarization inhomogeneous in the QW plane can be created, e.g., via DNP by optical grating technique [38–40]. In the case of macroscopic nuclear polarization, the interaction can be described as the Zeeman term

$$V(\boldsymbol{\rho}) = g\mu_B\,\boldsymbol{S}\cdot\boldsymbol{B}_n(\boldsymbol{\rho}), \tag{23}$$

with the effective nuclear (Overhauser) magnetic field

$$\boldsymbol{B}_n(\boldsymbol{\rho}) = \sum_\alpha(A_\alpha v_0 N_\alpha/g\mu_B)\int\overline{\boldsymbol{I}_\alpha(\boldsymbol{\rho},z)}\,\psi^2(z)dz, \tag{24}$$

which varies in the QW plane at a scale much larger than the crystal lattice constant. Here, μ_B is the Bohr magneton, g is the effective electron g factor, and the overbar denotes quantum mechanical averaging over the ensemble of nuclear wave functions.

The effective magnetic field, Eq. (23), produces a spin-dependent electron potential which causes scattering. For the effective field $\boldsymbol{B}_n(\boldsymbol{\rho})$ oriented along a certain axis, e.g., the

growth direction, the momentum relaxation time assumes the form

$$\tau_p^{-1} = \frac{m^*(g\mu_B)^2}{8\pi\hbar^3}\int_{-\pi}^{\pi}\langle \boldsymbol{B}_n(\boldsymbol{\rho})\cdot\boldsymbol{B}_n(\boldsymbol{\rho}')\rangle_{2k_F\sin\theta/2}(1-\cos\theta)d\theta, \tag{25}$$

where $\langle \boldsymbol{B}_n(\boldsymbol{\rho})\cdot\boldsymbol{B}_n(\boldsymbol{\rho}')\rangle_{\boldsymbol{q}}$ is the Fourier image of the spatial correlation function $\langle \boldsymbol{B}_n(\boldsymbol{\rho})\cdot\boldsymbol{B}_n(\boldsymbol{\rho}')\rangle$, k_F is the Fermi wave vector, and θ is the angle of scattering.

To estimate the momentum relaxation time we assume that the nuclear polarization is randomly distributed in the QW plane with the characteristic correlation length l and zero mean value. Then, for GaAs-based QWs with nuclear polarization $\overline{\boldsymbol{I}_\alpha} \sim 1$, $v_0\sum_\alpha A_\alpha N_\alpha \approx 0.1$ meV [28], Fermi wave vector $k_F = 10^6\,\mathrm{cm}^{-1}$, and correlation length $l \sim 1/k_F$, one obtains $\tau_p \sim 10^{-9}$ s. This τ_p is comparable to the momentum relaxation time in high-mobility structures. It indicates that strong spatially inhomogeneous spin polarization of nuclei can considerably affect electron transport in quantum wells and can be probed by electrical measurements. Spatially oscillating nuclear polarization created by optical grating technique may cause Bragg diffraction of electrons and has an even stronger impact on electron transport.

V. SUMMARY

To summarize, we have calculated the limitation of electron mobility in III–V quantum wells from the unavoidable source of disorder originating from fluctuations of nuclear spins. We have analyzed various spin configurations of the electron and nuclear subsystems and shown that the electron mobility determined by the electron-nuclear hyperfine interaction depends greatly on the spatial correlation of nuclear spins. While the electron mobility limited by the hyperfine interaction with uncorrelated nuclear spins is still a few orders of magnitude higher than that achieved in high-mobility quantum wells, nuclear spins that are spatially correlated and polarized at a macroscopic scale can considerably affect electron transport in modern high-mobility quantum wells.

ACKNOWLEDGMENTS

The work of S.A.T. was supported by the Russian Science Foundation (Project No. 14-12-01067). G.B. received support from the DFG within SFB767.

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