Weak localization in quantum wells with spin–orbit interaction

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The quantum interference correction to the conductivity is calculated for 2D electrons in a cubic A_3B_5 crystal with spin–orbit splitting by solving appropriate cooperon equation. The spin dependent vector-potential due to spin–orbit coupling leads to considerable changes compared to Larkin-Hikami-Nagaoka expression. © *1994 American Institute of Physics.*

Weak localization corrections to the conductivity of 2D structures in a magnetic field were obtained by Hikami *et al.*[1] in their pioneering work. Only the spin–orbit skew scattering mechanism (Elliot–Jaffet mechanism) of electron spin relaxation was considered as the origin of the spin–orbit effect on the conductivity. In subsequent studies of the weak localization the spin–orbit effects for 2D conductors without an inversion center were treated exclusively in terms of the Dyakonov–Perel spin relaxation time, in close analogy with the skew scattering effect (see, e.g., Refs. 2 and 3). Recently,[4–6] it was demonstrated that the spin–orbit interaction effect on the weak localization and universal conductance fluctuations should be considered as an effect of the spin-dependent vector potential, and important terms connected with this vector potential were shown to exist in the cooperon equation. Such an approach considerably changes the results[1,2] for spin–orbit coupling. In the present paper we study the anomalous magnetoresistance. Its experimental investigation is the most convenient tool for the examination of the weak localization effects,[3,7,8] and the improvement of theoretical formulas is important for the determination of various relaxation times and the spin–orbit splitting. For this purpose we solve here exactly the cooperon equation which is obtained by direct use of the Green's functions which explicitly include the spin–orbit terms in the Hamiltonian.

We consider here the quantum wells with the normal to the 2D plane in the (001) direction of the A_3B_5 cubic crystal. In that case the Hamiltonian for 2D electrons has the form (we assume $\hbar=1$)

$$H=\frac{k^2}{2m}+\vec{\sigma}\vec{\Omega}. \tag{1}$$

Here σ_i are the Pauli matrices and $\Omega_x=-\Omega_1\cos\varphi-\Omega_3\cos 3\varphi$, $\Omega_y=\Omega_1\sin\varphi-\Omega_3\sin 3\varphi$, $\Omega_1=\gamma k[k_z^2-(k^2/4)]$, $\Omega_3=\gamma(k^3/4)$, $\tan\varphi=(k_y/k_x)$, and $k^2=k_x^2+k_y^2$. Here $k_z^2=\int|\partial\psi/\partial z|^2dz$ is the mean square of the electron momentum in the direction perpendicular to the 2D plane, ψ is the electron wave function, k_x and k_y are the components of the in-plane electron momentum, and γ is the spin–orbit coupling constant. We assume anisotropic elastic scattering and introduce the probability of the scattering $W(\vartheta)$ per angle ϑ per unit time.

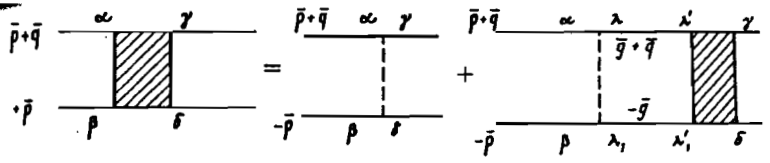

FIG. 1. Graphic representation of the cooperon equation.

The weak localization correction is expressed in terms of the cooperon amplitude $C(q,\vartheta,k_F)$, where q is a small total cooperon momentum, and ϑ is the angle defining the position of the electron momentum on the Fermi surface, $k=k_F$ (see, e.g., the review article[5]), which is defined by the graphical equation in Fig. 1. The Green's functions (heavy lines) entering the cooperon equation are expressed in terms of the Hamiltonian (1) and the elastic relaxation time τ_0:

$$G^+(k,\omega)=\frac{I}{\omega-(k^2/2m)-\vec{\sigma}\vec{\Omega}\pm(i/2\tau_0)}, \tag{2}$$

where $G^\pm$ is a 2×2 matrix in spin indices, I is a unit matrix, and

$$\frac{1}{\tau_0}=\int W(\vartheta)d\vartheta. \tag{3}$$

As usual, in weak localization theory the equation for the cooperon amplitude $C=C(q,\vartheta,k_F)$ can be solved by perturbation theory, assuming that $1/\tau_0$ is large compared to the spin–orbit energy splitting and v_Fq (v_F is the Fermi velocity). The cooperon amplitude can be expanded in Fourier harmonics of ϑ. It turns out that the first and third harmonics are small and can be expressed in terms of zero harmonic C_0. The substitution of higher-order harmonics in the zero harmonic equation gives the effective matrix equation for $C_0(k_F,q)$:

$$\hat{L}C_0=\frac{1}{2\pi\nu_0\tau_0}, \tag{4}$$

where

$$\hat{L}=\tau_0\left\{\frac{1}{\tau_\varphi}+\frac{1}{2}v_F^2q^2\tau_1+2(\Omega_1^2\tau_1+\Omega_3^2\tau_3)(1+\sigma_+\rho_-+\sigma_-\rho_+)\right.$$
$$\left.-\tau_1v_F\Omega_1[(\sigma_++\rho_+)\dot{q}_++(\sigma_-+\rho_-)q_-]\right\}. \tag{5}$$

Here we introduce the inverse phase relaxation time $1/\tau_\varphi$ as a cutoff at small q, the transport times

$$\frac{1}{\tau_1}=\int (1-\cos\theta)W(\theta)d\theta, \quad \frac{1}{\tau_3}=\int (1-\cos 3\theta)W(\theta)d\theta, \tag{6}$$

the density of states $\nu_0=m/2\pi$, $\sigma_\pm=\frac{1}{2}(\sigma_x\pm i\sigma_y)$, $\rho_\pm=\frac{1}{2}(\rho_x\pm i\rho_y)$ are the combinations of the Pauli matrices acting on the upper and lower spin indices of Fig. 1, respectively, I is the product of the unit matrices in the same basis, and $q_\pm=q_x\pm iq_y$.

The solution of Eq. (4) can be represented in the form

$$C^{\alpha\gamma}_{\beta\delta}(q)=\frac{1}{2\pi\nu_0\tau_0}\sum_\tau \frac{1}{E_\tau}\psi_{\tau,q}(\alpha,\beta)\psi^*_{\tau,q}(\gamma,\delta), \tag{7}$$

where $\psi_{\tau,q}$ and $E_\tau(q)$ are normalized eigenfunctions and eigenvalues of the operator $\hat{L}$:

$$\hat{L}\psi_\tau=E_\tau\psi_\tau. \tag{8}$$

These eigenfunctions can be classified by the value of the total spin momentum of two particles: antisymmetrical singlet $l=0$ $(r=0)$ and symmetrical $l=1$ $(r=1,2,3)$; in the latter case we use also the basis of the functions with integer spin momentum projection onto the Z axis, $\Phi_{l=1,m}$ $(m=1, 0, -1)$.

The quantum interference correction to the conductivity is proportional to (see, e.g., Ref. 2) the sum

$$S(q)=\sum_{\alpha,\beta} C^{\alpha\beta}_{\beta\alpha}=\frac{1}{2\pi\nu_0\tau_0}\left(-\frac{1}{E_0}+\sum_{\tau=1}^{3}\frac{1}{E_\tau}\right). \tag{9}$$

The singlet eigenvalue E_0 does not depend on the spin–orbit term

$$E_0=\left(Dq^2+\frac{1}{\tau_\phi}\right)\tau_0, \quad D=\frac{1}{2}v_F^2\tau_1.$$

The triplet eigenvalues can also be easily found by solving Eq. (8) (for the total momentum $l=1$) with

$$L=\tau_0\left[Dq^2+\frac{1}{\tau_\phi}+2(\Omega_1^2\tau_1+\Omega_3^2\tau_3)(2-J_z^2)-\tau_1 v_F\Omega_1\sqrt{2}(J_+q_++J_-q_-)\right], \tag{10}$$

where $\mathbf{J}$ is the angular momentum operator: $\mathbf{J}=\frac{1}{2}(\vec{\sigma}+\vec{\rho})$ and $J_\pm=1/\sqrt{2}(\sigma_\pm+\rho_\pm)$. It is convenient to express the sum of inverse eigenvalues in (8) directly in terms of the coefficients of secular equation. Such an approach gives us a possibility of finding a solution of the problem in the case of applied magnetic field. Using expression (8) for S, we obtain by standard procedure the weak localization correction to the conductivity without the magnetic field retaining only logarithmic terms

$$\Delta\sigma(0)=-\frac{e^2}{\pi}\nu_0\tau_0 D\int S(q^2)\frac{d^2q}{(2\pi)^2}$$
$$=-\frac{e^2}{2\pi^2\hbar}\left\{-\frac{1}{2}\ln\frac{\tau_1}{\tau_\varphi}+\ln\left(\frac{\tau_1}{\tau_\varphi}+\frac{\tau_1}{\tau_{Sxx}}\right)+\frac{1}{2}\ln\left(\frac{\tau_1}{\tau_\varphi}+\frac{\tau_1}{\tau_{Szz}}\right)\right\}. \tag{11}$$

Here $1/\tau_{Sxx}=1/\tau_{Syy}=1/2\tau_{Szz}=2(\Omega_1^2\tau_1+\Omega_3^2\tau_3)$, where τ_{Sii} are the spin relaxation times defined by the equation[7,8] $dS_i/dt=-(S_i/\tau_{Sii})$. From expression (11) we see that with the logarithmic accuracy the spin-dependent vector potential terms in the cooperon equation are not essential for the temperature-dependent corrections to the conductivity.[6]

In the presence of a magnetic field B, the quantities $q_\pm$ and q^2 in Eqs. (5) and (10) are defined by gauge invariance and become $q_+=\sqrt{2}Sa$ and $q_-=\sqrt{2}Sa^+$, where $S^2=2eB/c$, and a and a^+ are the operators which increase or decrease the number n of the Landau level of the wave function F_n:

$$(a^+a)F_n=(n+\tfrac{1}{2})F_n, \quad aF_n=\sqrt{n}F_{n-1}, \quad a^+F_n+\sqrt{n+1}F_{n+1}.$$

The eigenvalue $E_0(n)$ does not depend on the spin–orbit interaction and is given in Ref. 1. According to Eqs. (8) and (10), the solution $\vec{\psi}(n)$ in the basis of the functions $\Phi_{l=1,m}$ with the momentum projection m has the form

$$\vec{\psi}_1(n)=[f_{1,\tau}(n)F_{n-2},\ f_{0,\tau}(n)F_{n-1},\ f_{-1,\tau}(n)F_n]. \tag{12}$$

Substitution of (12) in Eqs. (8) and (10) gives the system of algebraic linear equations for the determination of $f_{i\tau}$, and the determinant of the appropriate matrix gives the secular equation for the eigenvalues $E_\tau(n)$ $(r=1,2,3)$. In the case $n=0$, F_{n-1} and F_{n-2} must be set to zero, and there is only one eigenvalue $E_1(0)$. In the case $n=1$, F_{n-2} must be set to zero, and there are two eigenvalues, $E_1(1)$ and $E_2(1)$, which are defined by an appropriate quadratic equation. For all other $n\geqslant 2$ there are three eigenvalues $E_\tau(n)(r-1,2,3)$, which are defined by a cubic equation. As in the case without a magnetic field, the sum (9) can be expressed directly in terms of the coefficients of secular equation without solving it. Being short on space, we give the final expression for the conductivity correction:

$$\Delta\sigma(B)=-\frac{e^2}{4\pi^2\hbar}\left\{\frac{1}{a_0}+\frac{2a_0+1+(H_{SO}/B)}{a_1[a_0+(H_{SO}/B]-(2H'_{SO}/B)}\right.$$
$$-\sum_{n=1}^{\infty}\left[\frac{3}{n}-\frac{3a_n^2+2a_n(H_{SO}/B)-1-2(2n+1)(H'_{SO}/B)}{[a_n+(H_{SO}/B)]a_{n-1}a_{n+1}-2(H'_{SO}/B)[(2n+1)a_n-1]}\right.$$
$$\left.\left.+2\ln\frac{H_{t\tau}}{B}+\psi\left(\frac{1}{2}+\frac{H_\varphi}{B}\right)+3C\right\}\right., \tag{13}$$

where

$$a_n=n+\frac{1}{2}+\frac{H_\varphi}{B}+\frac{H_{SO}}{B}, \quad H_\varphi=\frac{c\hbar}{4eD\tau_\varphi}, \quad H_{SO}=\frac{c\hbar}{4eD}(2\Omega_1^2\tau_1+2\Omega_3^2\tau_3),$$
$$H'_{SO}=\frac{c\hbar}{4eD}2\Omega_1^2\tau_1, \quad H_{t\tau}=\frac{c\hbar}{4eD\tau_1}, \quad \psi(1+z)=-C+\sum_{n=1}^{\infty}\frac{z}{n(n+z)}, \tag{14}$$

and C is the Euler constant. If we omit terms containing H'_{SO}/B, we obtain the Hikami-Larkin-Nagoaka expression from (13):

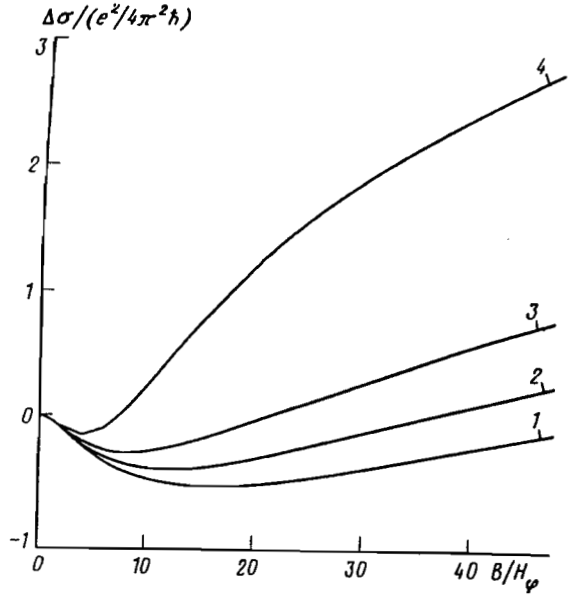

FIG. 2. Magnetic field dependence of the conductivity corrections in units of $e^2/4\pi^2\hbar$ for $H_{SO}/H_\varphi=4$, and $H'_{SO}/H_{SO}=0$ (*1*), 0.25 (*2*), 0.5 (*3*), 1 (*4*).

$$\Delta\sigma(B)-\Delta\sigma(0)=\frac{e^2}{2\pi^2\hbar}\left\{\psi\left(\frac{1}{2}+\frac{H_\varphi}{B}+\frac{H_{SO}}{B}\right)+\frac{1}{2}\psi\left(\frac{1}{2}+\frac{H_\varphi}{B}+\frac{2H_{SO}}{B}\right)\right.$$
$$\left.-\frac{1}{2}\psi\left(\frac{1}{2}+\frac{H_\varphi}{B}\right)-\ln\frac{H_\varphi+H_{SO}}{B}-\frac{1}{2}\ln\frac{H_\varphi+2H_{SO}}{B}+\frac{1}{2}\ln\frac{H_\varphi}{B}\right\}. \quad (15)$$

However, for the magnetic field $B\sim H_{SO}$, Eqs. (13) and (15) are numerically different. Figure 2 shows the dependence $\Delta\sigma(B)-\Delta\sigma(0)$ calculated in accordance with Eq. (13) for $H_{SO}/H_\phi=4$, $H'_{SO}/H_{SO}=1$, 1/2, 1/4, and $H'_{SO}=0$ when (15) is applicable. The real values of H'_{SO}/H_{SO} are close to 1. We see that in this case the value of $\Delta\sigma(B)-\Delta\sigma(0)$ for B larger than H_φ and H_{SO} essentially increases. This is explained by the fact that for nonvanishing H'_{SO}, according to (13), $\Delta\sigma(0)$ contains, in addition to the logarithmic term (11), a large additional contribution which also vanishes in a strong magnetic field.

The other difference (besides the difference in τ_1, τ_3), compared with Refs. 2 and 3, is in the value of H_{SO} in (13) and (15), which is twice as large in terms of the same Hamiltonian. The relaxation time introduced in Refs. 2 and 3, $1/\tau_{SOi}=\langle\Omega_i^2\rangle\tau$ (here $\langle\Omega_i^2\rangle$ is the average over the Fermi surface) by definition does not coincide with the spin relaxation times which are[9,10]

$$\frac{1}{\tau_{Sii}}=2(\langle\Omega^2\rangle-\langle\Omega_i^2\rangle)\tau.$$

[For comparison of the results we recall that in Refs. 9 and 10 the spin–orbit Hamiltonian is in the form $H_{SO}=1/2\vec{\sigma}\vec{\Omega}$, instead of (1)]. Similar remark pertains to the 3D case which was considered in Ref. 2.

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