Role of quantum contributions in magnetoconductance behavior at low temperatures in iridate films

A. L. Danilyuk[1], D. A. Podryabinkin[1], A. B. Filonov[1], G. A. Ovsyannikov[2], G.D. Ulev[2,3], K. Y. Constantinian[2], D. B. Migas[1,4,*]

[1]*Belarusian State University of Informatics and Radioelectronics, P. Browka 6, Minsk 220013, Belarus*

[2] *Kotel'nikov Institute of Radio Engineering and Electronics of RAS, Moscow 125009, Russia*

[3]*Moscow Institute of Physics and Technology (National Research University), Dolgoprudny, Moscow oblast, 141701 Russia*

[4]*National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe Shosse 31, 115409, Moscow, Russia*

* Contact person: migas@bsuir.by

Supplementary materials

The resistance of $SrIrO_3$ films on $SrTiO_3$ versus temperature shows non-trivial behavior.

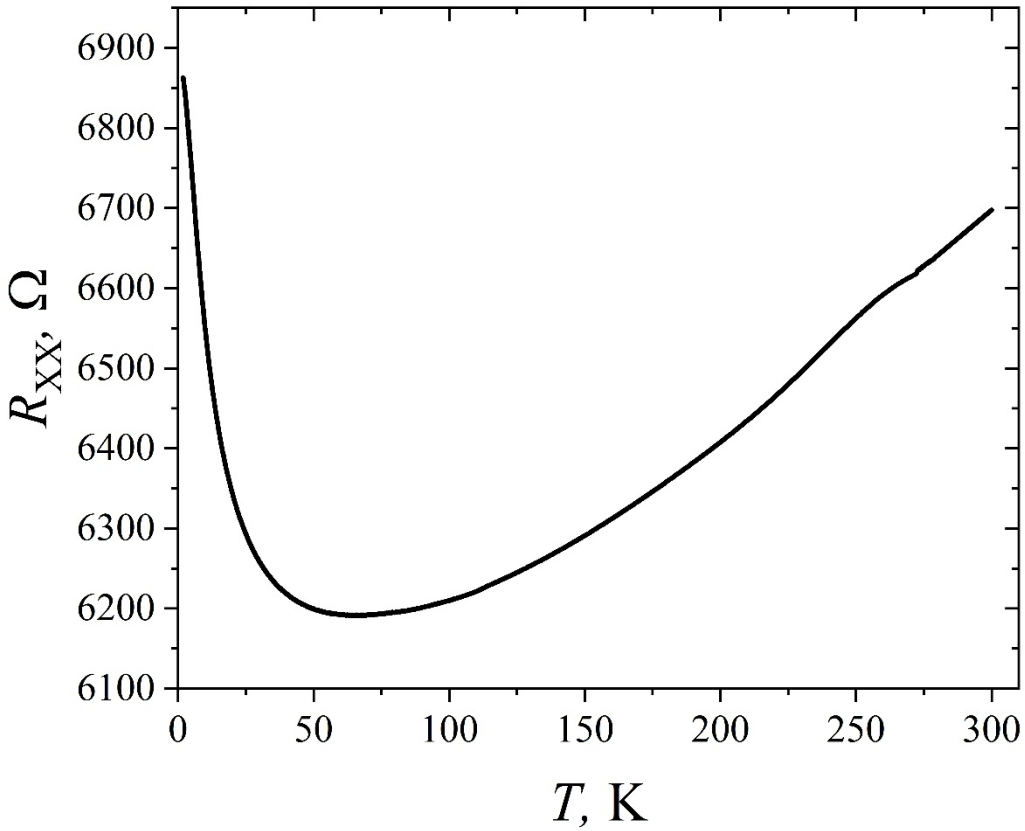

Figure S1. Resistance versus temperature of thin $SrIrO_3$ film on $SrTiO_3$ substrate in the extended temperature range from 1.86 to 300 K. The data in the low-temperature region below 30 K is the object of the present study.

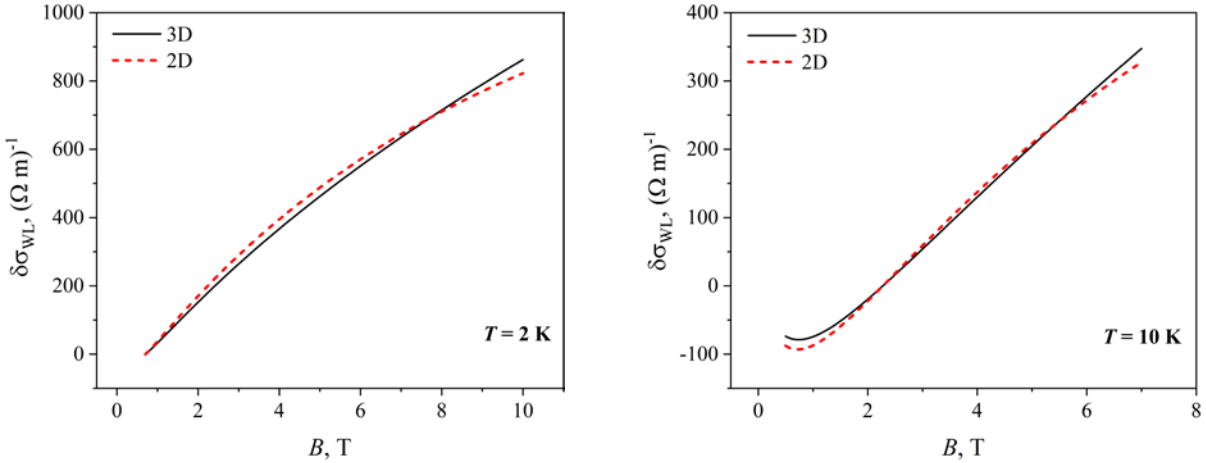

Figure S2. Comparison of the 2D and 3D quantum contributions of $\delta\sigma_{WL}$ at different temperatures.

The quantum contribution theory is valid for a degenerate electron gas in the case of a metal-like conductance for a weak disordered system. In accordance to the Ioffe-Regel criterion [1] the electron mean free path (l) is larger than electron wave length ($1/k_F$), *i.e.* $k_F l > 1$. For the 50 nm thick $SrIrO_3$ film (close to our case) [2] the electron concentration (n_e) was 3×10^{20} cm^{-3}, the impulse relaxation time (τ) was 50 fs and the Fermi velocity (v_F) was estimated to be (1.2 – 5.0) 10^5 m/s [3,4]. Thus, the Fermi wave number ($k_F = (3\pi^2 n_e)^{1/3}$) is 2.07×10^9 m^{-1}, and the electron free pass length ($l = v_F\times\tau$) is 5 – 25 nm, *i.e.* the minimal value of $k_F l$ is 10.4 indicating that the Ioffe-Regel criterion is fulfilled.

The estimated Hartree factor value (F), defined by the ratio of the exchange term to Hartree contribution one, clearly indicates the presence of the exchange interaction. At the same time, the ratio of the Thomas–Fermi scattering parameter (κ_{TF}) to the Fermi wave number (k_F) is decreased with the temperature raise, which, in its turn, within the Thomas–Fermi Theory of Screening for a free electron gas ($T << T_F$), leads to an increase in the Coulomb scattering contribution to the conductivity (the screening radius is decreased). However, that does not correlate with the raise in the diffusion coefficient and conductivity in our case. On the other hand, the ratio of the Kleinman–Langreth scattering parameter (κ_S), which in contrast to the κ_{TF} parameter accounts for the exchange contribution to the Coulomb repulsion as well, to the Fermi wave number (k_F) is increased with the temperature. So, the latter fact along with the Hartree parameter decrease indicates that the Coulomb scattering contribution to the conductivity also drops, which correlates well with the obtained experimental data. Thus, such the k_F/κ_{TF} and κ_S/k_F ratio values are an indirect proof of the $SrIrO_3$ electron system to be a non-Fermi liquid.

As seen from the Table, the dephasing or inelastic scattering time (τ_i) does not change with temperature, whereas the subsequent length (L_i) is increased with temperature due to the raise in the diffusion coefficient. On the whole, the inelastic scattering length for the electron transport under weak localization [5] either does not change or decreases as $L_i \sim 1/T^{p/2}$ [6] with the temperature raise. However, in our case these tendencies do not hold due to the anti-localization effects. Also note, the Equivalent fields of inelastic scattering B_i are reduced from 1.373 (2 K) to 1.030 (10 K) mT.

The spin-orbit scattering is most significant (Fig. 7) when the weak localization is dominated over the weak anti-localization (*i.e.* at $\delta\sigma_{WL}<0$) at the fields lower than 0.605 (2 K) and 2.26 (10 K) T in our case. The spin-orbit scattering time (τ_{so}) is considerably reduced (about 3.4 times) with temperature raise, and the Equivalent fields of the spin-orbit scattering ($B_{SO}=\hbar/(4eD\tau_{so})$,) are increased from 92 (2 K) to 234 (10 K) mT. The appropriate Rashba spin-orbit coupling coefficient ($\alpha=(q\hbar^3 B_{SO})^{1/2}/m_e$) ($q$ to be the electron charge, m_e to be the electron

effective mass, and B to be the magnetic field induction) is increased 1.6 times, and this result correlates well with the B_{SO} measured experimental data in the low-temperature region [7,8]. The B_{SO} and Rashba coefficient raise was explained to the Lande factor drop with temperature raise [7,8] because of the strong spin-orbit coupling. This effect can be affected by the lattice thermal expansion in addition to the Coulomb interaction energy decrease with temperature raise that leads, in its turn, to the $SrIrO_3$ band gap shrinkage [8]. The appearance of the band gap in $SrIrO_3$ has been theoretically observed under some conditions [9]. The other possible model based on the scattering by paramagnetic impurities was also proposed [10]. The effect of spin-orbit scattering time reduction can be connected with anisotropy of spin-orbit scattering on magnetic moments [11] and leads to the anomalous Hall effect [11-14] due to the spin-orbit scattering of conductive electrons by magnetic moment fluctuations of inner-shell electrons when the interaction of electrons with "magnetic" atoms plays a dominant role.

The weak localization is caused by an interference of wave functions of electrons passed the same way in direct and reverse directions. Such the interference depends on the total spin (S) of these two electron waves, which can interfere in a constructive or destructive way. The spin-orbit interaction by the spin relaxation mechanism significantly modifies quantum contributions to the conductivity defined by the localization [15], as well as the electron-electron interaction [16,17] in disordered electron systems. Upon the spin-orbit scattering the single electron spin is no longer a "good" quantum number, but unlike the spin-flip scattering the time reverse symmetry is preserved. In the weak localization theory (defined by the mechanism of the interference of electron waves scattered on impurities) the sign of the contribution to the conductivity depends on the relation between the inelastic scattering time (τ_i) and the spin-orbit scattering time (τ_{so}). The spin relaxation is negligible at $\tau_{so} \gg \tau_i$, and the temperature dependence of the conductivity is defined by carrier weak localization. However, if $\tau_{so} \ll \tau_i$, the quantum contribution to the conductivity can be either a negative (weak localization) or positive (anti-localization) non negligible value [15,18-21].

In the case of spin-orbit scattering, the weak localization effect (conductivity decrease) is defined only by the interference of waves of triplet states with $|S|=1$, whereas the interference of waves of singlet states with $S=0$ leads to the anti-localization (conductivity increase). The interaction of particles with opposite spin ($S=0$) is only essential for the Cooper's channel. The channel existence is determined not only by the preservation of a number of particles with a defined energy, but also by the time reverse invariance. At the same time, the spin-orbit electron scattering does not affect the contribution caused by the Coulomb interaction, as far as the time invariance is preserved in the presence of the scattering. Note, such behavior is observed only at the absence of an external magnetic field. The $\phi_3(B)$ function increases with the magnetic field

as $\ln(2qBD/\pi k_B T)$ at $2qBD/\pi k_B T >> 1$. The behavior of the $g(T,B)$ constant interaction function (obtained for the F_σ parameter, the diffusion coefficient D from the Table and the Debye temperature of 326 K [22]) with respect to the magnetic field, as, is shown in Fig. S3.

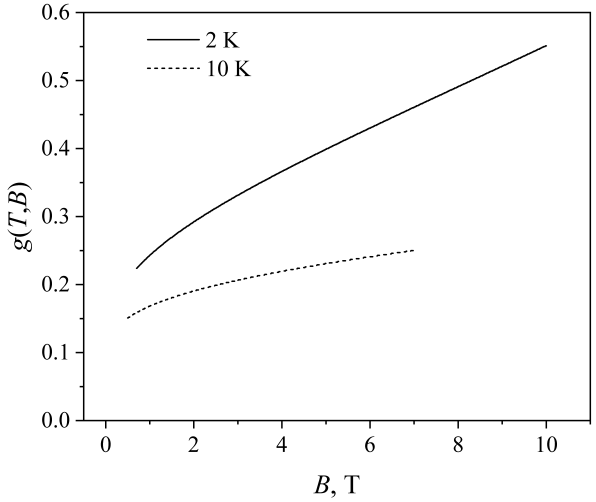

Figure S3. The $g(T,B)$ constant interaction function versus the magnetic field induction at different temperatures.

SM References

[1] A.F. Ioffe, A.R. Regel, Non-crystalline, amorphous, and liquid electronic semiconductors. Prog. Semicond. 4 (1960) 237 - 291.

[2] K. Sen, D. Fuchs, R. Heid, K. Kleindienst, K. Wolff, J. Schmalian, M. Le Tacon, Strange semimetal dynamics in $SrIrO_3$. Nat. Commun. 11 (2020) Article number 4270. https://doi.org/10.1038/s41467-020-18092-6.

[3] N. Manca, D.J. Groenendijk, I. Pallecchi, C. Autieri, L.M.K. Tang, F. Telesio, G. Mattoni, A. McCollam, S. Picozzi, A.D. Caviglia, Balanced electron-hole transport in spin-orbit semimetal $SrIrO_3$ heterostructures. Phys. Rev. B 97 (2018) 081105(R). https://doi.org/10.1103/PhysRevB.97.081105.

[4] A. Yamasaki, H. Fujiwara, S. Tachibana, D. Iwasaki, Y. Higashino, C. Yoshimi, K. Nakagawa, Y. Nakatani, K. Yamagami, H. Aratani, O. Kirilmaz, M. Sing, R. Claessen, H. Watanabe, T. Shirakawa, S. Yunoki, A. Naitoh, K. Takase, J. Matsuno, H. Takagi, A. Sekiyama, Y. Saitoh, Three-dimensional electronic structures and the metal-insulator transition in Ruddlesden-Popper iridates. Phys. Rev. B 94 (2016) 115103. https://doi.org/10.1103/PhysRevB.94.115103.

[5] P. Sheng, Introduction to wave scattering: Localization and mesoscopic phenomena (Springer-Verlag, Berlin, Heidelberg, 2006), 333 p. https://doi.org/10.1007/3-540-29156-3.

[6] P.A. Lee, T.V. Ramakrishnan, Disordered electronic systems, Rev. Mod. Phys. 57 (1985) 287 – 337. https://doi.org/ 10.1103/RevModPhys.57.287.

[7] L. Zhang, B. Pang, Y.B. Chen, Y. Chen, Review of spin–orbit coupled semimetal $SrIrO_3$ in thin film form. Crit. Rev. Solid State Mater. Sci. 43 (2018) 367 - 391. https://doi.org/ 10.1080/10408436.2017.1358147.

[8] L. Zhang, Y.B. Chen, J. Zhou, S.-T. Zhang, Z.-B. Gu, S.-H. Yao, Y.-F. Chen, Sensitively temperature-dependent spin–orbit coupling in $SrIrO_3$ thin films, . J. Phys. Soc. Jpn. 83 (2014) 054707. https://doi.org/10.7566/JPSJ.83.054707.

[9] P. Liu, C. Franchini, Advanced first-principle modeling of relativistic Ruddlesden-Popper strontium iridates. Appl. Sci. 11 (2021) 2527. https://doi.org/10.3390/app11062527.

[10] L. Fruchter, O. Schneegans, Z.Z. Li, Anisotropy and interaction effects of strongly strained $SrIrO_3$ thin films. J. Appl. Phys. 120 (2016) 075307. https://doi.org/10.1063/1.4960700.

[11] A.F. Barabanov, Yu.M. Kagan, T.V. Khabarova, L.A. Maksimov, A.V. Mikheyenkov, The Hall effect and its analogs. Phys.-Usp. 58 (2015) 479 - 488. https://doi.org/ 10.3367/UFNr.0185.201505b.0479.

[12] J.M. Luttinger, Theory of the Hall effect in ferromagnetic substances. Phys. Rev. 112 (1958) 739 - 751. https://doi.org/ 10.1103/physrev.112.739.

[13] N. Nagaosa, J. Sinova, S. Onoda, A.H. MacDonald, N.P. Ong, Anomalous Hall effect. Rev. Mod. Phys. 82 (2010) 1539 - 1592. https://doi.org/10.1103/revmodphys.82.1539.

[14] L.E. Gurevich, I.N. Yassievich, Low-temperature transport properties of metals with paramagnetic impurities. JETP 20 (1965) 922 - 928. http://jetp.ras.ru/cgi-bin/dn/e_020_04_0922.pdf

[15] S. Hikami, A.I. Larkin, Y. Nagaoka, Spin-orbit interaction and magnetoresistance in the two dimensional random system. Prog. Theor. Phys. 63 (1980) 707 - 710. https://doi.org/10.1143/PTP.63.707.

[16] S.V. Iordanskii, Yu.B. Lyanda–Geller, G.E. Pikus, Weak localization in quantum wells with spin-orbit interaction. JETP Lett. 60 (1994) 206 - 210.
http://www.jetpletters.ru/ps/1323/article_20010.pdf

[17] W. Knap, C. Skierbiszewski, A. Zduniak, E. Litwin–Staszewska, D. Bertho, F. Kobbi, J.L. Robert, G.E. Pikus, F.G. Pikus, S.V. Iordanskii, V. Mosser, K. Zekentes, Yu.B. Lyanda–Geller, Weak antilocalization and spin precession in quantum wells. Phys. Rev. B 53 (1996) 3912 - 3924. https://doi.org/10.1103/physrevb.53.3912.

[18] A. Kawabata, Theory of negative magnetoresistance I. Application to heavily doped semiconductors. J. Phys. Soc. Jpn. 49 (1980) 628 - 637. https://doi.org/ 10.1143/JPSJ.49.628.

[19] G. Bergmann, Weak localization in thin films: a time-of-flight experiment with conduction electrons. Phys. Rep. 107 (1984) 1 - 58. https://doi.org/10.1016/0370-1573(84)90103-0.

[20] B.L. Altshuler, D. Khmel'nitskii, A.I. Larkin, P.A. Lee, Magnetoresistance and Hall effect in a disordered two-dimensional electron gas. Phys. Rev. B 22 (1980) 5142 - 5153. https://doi.org/10.1103/PhysRevB.22.5142.

[21] D.V. Baxter, R. Richter, M.L. Trudeau, R.W. Cochrane, J.O. Strom-Olsen, Fitting to magnetoresistance under weak localization in three dimensions. J. Physique. 50 (1989) 1673 - 1688. https://doi.org/10.1051/jphys:0198900500130167300.

[22] G. Cao, V. Durairaj, S. Chikara, L.E. DeLong, S. Parkin, P. Schlottmann, Fermi-liquid behavior in nearly ferromagnetic $SrIrO_3$ single crystals. Phys. Rev. B 76 (2007) 100402(R). https://doi.org/10.1103/PhysRevB.76.100402.