Intrinsic spin Hall effect at asymmetric oxide interfaces: Role of transverse wave functions

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Outline

Motivations

1. Experiments: 2DEG at interface between two oxides (LAO/STO)
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   - S. Thiel, G. Hammerl, A. Schmehl, C. W. Schneider, and J. Mannhart, Science **313**, 1942 (2006).
   - M. Huijben et al., Nat. Mater. **5**, 556 (2006).
   - E. Dagotto, Science **318**, 1076 (2007).
   - Rashba SOC: $\hbar\alpha \sim 5 \times 10^{-2}\mathrm{eV}\mathring{A}$, A. D. Caviglia et al., Phys. Rev. Lett. **104**, 126803 (2010).
2. Theory: Non uniform Rashba SOC
   - Random Rashba: V. K. Dugaev,M. Inglot, E. Ya. Sherman, and J. Barnas, Phys. Rev. B 82, 121310(R) (2010).
   - A finite-tickness 2DEG: X. Wang, J. Xiao, A. Manchon, and S. Maekawa, Phys. Rev. B **87**, 081407 (2013).
   - e-e Interaction controlled Rashba SOC: S. Caprara, F. Peronaci, and M. Grilli, Phys. Rev. Lett. **109**, 196401 (2012).

General aim

Move away from the strictly two-dimensional electron gas model

Symmetry arguments

The Rashba Hamiltonian for the 2DEG

$$H = \frac{p^2}{2m} + \alpha\, \hat{\mathbf{e}}_z \times \sigma \cdot \mathbf{p} + V(\mathbf{r})$$

Why SHE is bound to be zero?

(By the way: I have been telling you this since 2005 and may be you are bored to listen to me again!)
Operatorial identity:

$$\frac{\mathrm{d}\hat{s}^y}{\mathrm{d}t} = -\frac{2m\alpha}{\hbar}\frac{\hat{p}_y}{m}\hat{s}^z$$

After averaging over the ground states

$$\frac{\mathrm{d}s^y}{\mathrm{d}t} = -\frac{2m\alpha}{\hbar} J_y^z$$

In static circumstances the spin current is bound to be zero!

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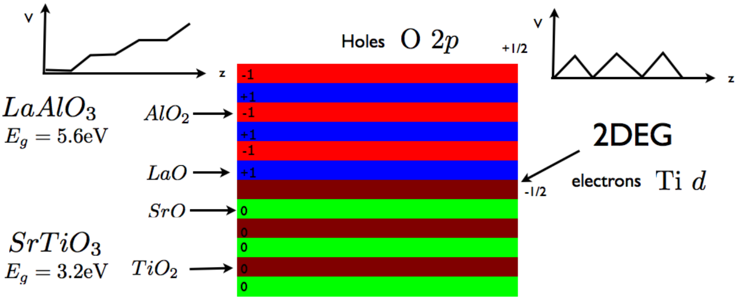
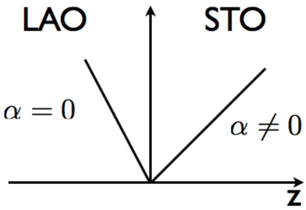
- E. G. Mishchenko, A. V. Shytov, and B. I. Halperin, Phys. Rev. Lett. **93**, 226602 (2004). R. Raimondi and P. Schwab, Phys. Rev. B **71**, 033311 (2005). A. Khaetskii, Phys. Rev. Lett. **96**, 056602 (2006).

Model





1. Stronger attraction to the interface on Al side due to reduced screening
2. Asymmetric SOC: Ti vs Al
3. Strong simplification: ignore the multi-band structure (for more details: Bistritzer et al. PRB **83**, 115114 (2011); Khalsa and MacDonald PRB **86**, 125121 (2012); Khalsa et al. arxXiv:1301:2784)

Model in formal terms

The Hamiltonian

$$H = \sum \left\{ \frac{\mathbf{p}^2}{2m} - \frac{\hbar^2}{2m}\frac{d^2}{dz^2} + V(z) - \frac{\lambda_c^2}{\hbar} V'(z)\Theta(z)[p_x\sigma_y - p_y\sigma_x] + V_{imp}(\mathbf{r}) \right\}$$

- $\mathbf{p} = (p_x, p_y)$ momentum operator in the plane of the quantum well
- effective Compton wavelength $\lambda_c \sim 0.7$ Å
- 2DEG (pure Rashba SOC) recovered as limiting case for $r \to \infty$

$$V(z) = \begin{cases} Fz & z > 0 \\ -rFz & z < 0 \end{cases}$$

- Quantum numbers: in-plane wavevector $\mathbf{k}$, spin index λ, subband index n

$$\psi_{n\mathbf{k}\lambda}(\mathbf{r}, z) = \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{\mathscr{A}}} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i\lambda e^{i\theta_{\mathbf{k}}} \end{pmatrix} f_{n\mathbf{k}\lambda}(z)$$

Notice: z-dependence of SOC implies $\mathbf{k}$-dependence of subband wavefunctions!

Symmetry arguments again

Why a non-zero SHC is possible?

- As for the 2DEG, there is an identity leading to

$$\frac{\mathrm{d}s^y}{\mathrm{d}t} = -\frac{2\lambda_c^2}{\hbar}\langle V'(z)\Theta(z)\hat{p}_y\sigma^z\rangle$$

- The standard argument does not apply since

$$\langle V'(z)\Theta(z)\hat{p}_y\sigma^z\rangle \neq \langle V'(z)\Theta(z)\rangle\langle\hat{p}_y\sigma^z\rangle \propto J_y^z$$

- The spin current vanishes only for $z > 0$, but nothing can be said about $z > 0$. A calculation is needed

Important parameters

- natural units: length $\ell = (\hbar^2/2mF)^{1/3}$, energy $F\ell$
- $\alpha = (\lambda_c/\ell)^2 \sim 1$ effective dimensionless SOC constant
- Question: to what order there is an effect?

Solution of the model

Analytic results in terms of the Airy function

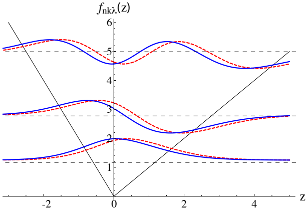
$$f_{k\lambda}(z) = Z \times \begin{cases} \dfrac{Ai(z-\varepsilon_{\mathbf{k}\lambda}-\lambda\alpha k)}{Ai(-\varepsilon_{k\lambda}-\lambda\alpha k)} & (z \geq 0) \\ \dfrac{Ai(-zr^{1/3}-\varepsilon_{k\lambda}r^{-2/3})}{Ai(-\varepsilon_{\mathbf{k}\lambda}r^{-2/3})} & (z < 0) \end{cases}$$

Eigenvalues $E_{n\mathbf{k}\lambda} = k^2 + \varepsilon_{n\mathbf{k}\lambda}$ obtained by imposing continuity of the derivative

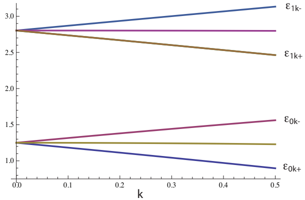
$$\frac{Ai'(-\varepsilon_{k\lambda} - \lambda\alpha k)}{Ai(-\varepsilon_{k\lambda} - \lambda\alpha k)} = -r^{1/3}\frac{Ai'(-\varepsilon_{k\lambda}r^{-2/3})}{Ai(-\varepsilon_{k\lambda}r^{-2/3})},$$

Important remark

The qualitative features of the **k**-dependence of the wavefunctions $f_{n\mathbf{k}\lambda}(z)$ can be studied by perturbation theory in $\lambda\alpha k$

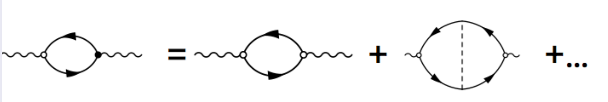


$\lambda = 1$ $\lambda = -1$



Evaluation of the Spin Hall Conductivity

The Kubo formula



$$[\sigma_{SH}]^z_{yx} = -e \lim_{\omega \to 0} \frac{1}{\omega} \int_{-\infty}^{\infty} \frac{\mathrm{d}\varepsilon}{2\pi} \mathrm{Tr}\left\{ \hat{\gamma}^z_y G(\varepsilon_+) \hat{\gamma}_x G(\varepsilon_-) \right\},$$

- Spin vertex $\hat{\gamma}^z_y = k_y \sigma^z$
- Charge vertex $\hat{\gamma}_x = -\alpha \Theta(z) \sigma^y$
- Vertex corrections due to standard impurity scattering

$$\hat{\Gamma}_x = \tilde{\gamma}_x + \frac{1}{2\pi N_0 \tau} \sum_{\mathbf{k}'} G^R_{\mathbf{k}'} \hat{\Gamma}_x G^A_{\mathbf{k}'}$$

$$\tilde{\gamma}_x = -\alpha \Theta(z) \sigma^y + \frac{1}{2\pi N_0 \tau} \sum_{\mathbf{k}'} G^R_{\mathbf{k}'} \, 2k'_x \, G^A_{\mathbf{k}'}$$

Classification of contributions

Due to the subband index, there are are **intra**-band and **inter**-band contributions to the SHC

The bare bubble contribution with Fermi level in the lowest ($n = 0$) subband

$$[\sigma_{SH}]^z_{yx} = -\frac{e}{4\pi}\sum_n \left[\int_0^{k_{F+}} \frac{|\langle f_{n\mathbf{k}-}|f_{0\mathbf{k}+}\rangle|^2}{\varepsilon_{0\mathbf{k}+} - \varepsilon_{n\mathbf{k}-}} kdk + \int_0^{k_{F-}} \frac{|\langle f_{n\mathbf{k}+}|f_{0\mathbf{k}-}\rangle|^2}{\varepsilon_{0\mathbf{k}-} - \varepsilon_{n\mathbf{k}+}} kdk \right]$$

Why inter-band terms?

They arise because wavefunctions of the same wave vector **k** and *opposite helicity* are not mutually orthogonal even when their subband indices differ

What about vertex corrections?

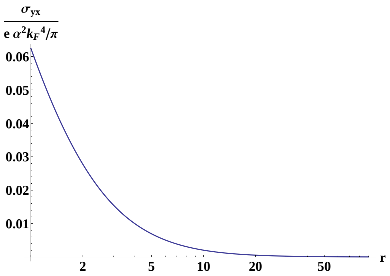
In the standard 2DEG case with Rashba SOC the vertex corrections cancel the bare bubble contribution so to satisfy the operatorial identity

1. Are vertex corrections important in this case?
2. Do they behave differently for inter- and intra-band contributions?

Results for inter-band contribution

Analytical expression for the bare bubble

$$[\sigma_{SH}^{\text{inter}}]_{yx}^{z} = -\frac{e}{\pi}\alpha^2 k_F^4 \sum_{n\neq 0} \frac{|p_{no}|^2}{(\varepsilon_0 - \varepsilon_n)^3}$$



Vertex corrections unimportant for inter-band terms!

Bare bubble terms originate from inter-band transitions with simultaneous flipping of the spin. Vertex corrections are due to processes where, first, the inter-band transition occurs without changing the spin, followed by a spin flip in the same subband (or the other way around). This costs energy for large enough subband separation.

Analysis of vertex corrections for intra-band contribution

A methodology remark

The presence of the Airy functions in the solution of the model requires the use of numerical approximations, which render delicate the investigation of **exact** cancellations between different terms. As a strategy, by using perturbation theory, we evaluate the energy eigenvalues in powers of $\lambda\alpha k$

$$E_{0k\lambda} = k^2 + e_1(\alpha k)\lambda + e_2(\alpha k)^2 + e_3(\alpha k)^3\lambda + \dots$$

The expression of the coefficients e_i can then also checked numerically by using Mathematica

The intra-band vertex $\langle 0\mathbf{k}\lambda|\tilde{\gamma}_x|0\mathbf{k}\bar{\lambda}\rangle$

- the bare matrix element

$$\frac{1}{2k}\left(E_{0k\lambda} - E_{0k\bar{\lambda}}\right) = \lambda\alpha e_1 + \lambda\alpha^3 e_3 k^2$$

- the correction

$$\frac{k_\lambda N_\lambda}{2N_0} - \frac{k_{\bar{\lambda}} N_{\bar{\lambda}}}{2N_0} = -\lambda\alpha e_1 + 2\lambda\alpha^3\left(e_1 e_2 - e_3 k_F^2\right)$$

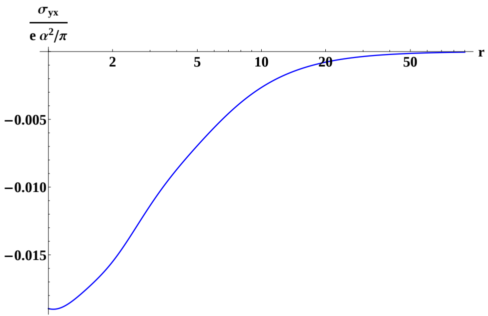
Results for intra-band contribution to SHC

Analytical expression

To order α^1, the vertex corrections cancel the bare bubble, but not to order α^3, hence cancellation is not a general feature as guessed on the basis of the operatorial identity

$$\left[\sigma_{SH}^{intra}\right]_{yx}^{z} = -\frac{e}{4\pi}\left\{\left(1-\frac{m}{m^*}\right)+\frac{\alpha^2 k_F^2}{2p_{00}}\left[\sum_{n,m\neq 0}\frac{p_{0n}p_{nm}p_{m0}}{(\varepsilon_n-\varepsilon_0)(\varepsilon_m-\varepsilon_0)}-\sum_{n\neq 0}\frac{|p_{0n}|^2}{(\varepsilon_n-\varepsilon_0)^2}\right]\right\}$$

Notice that it vanishes in the Rashba limit ($r \to \infty$)



Conclusions and acknowledgements

- Prediction of finite intrinsic SHC in 2DEG at oxides interfaces
- General model for taking into account finite tickness and $\hat{\mathbf{z}}$-dependence of the SOC away from the pure Rashba limit in strictly two dimensions
- Development of general strategy to deal with vertex corrections in non-easily analytically tractable situations

Collaborators

- Lorien H. Hayden (Columbia, USA)
- Michael Flatté (Iowa City, USA)
- Giovanni Vignale (Columbia, USA)

References

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Thank you for your attention!