SPIN AND CHARGE EFFECTS IN ONE AND TWO DIMENSIONAL SYSTEMS WITH SPIN-ORBIT INTERACTION

A Numerical Perspective

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OUTLINE

- Mesoscopic Quantum Transport Picture
- Longitudinal and Spin-Hall Conductances in 1D and 2D systems
- Time-Dependent Algorithms
- Edge Spin Accumulation
- Conclusions

THE SPIN HALL EFFECT AND THE <u>SPIN ORBIT</u> <u>INTERACTION (SOI)</u>



QUESTIONS

1. Robustness under disorder

*Cancellation of the effect in infinite 2D systems in the presence of infinitesimal amounts of disorder

- 2. Proper definition of the spin current
- 3. The universality of the transverse conductivity
- 4. Scaling with the dimensionality of the sample

Experiments are done in finite size samples

Preliminary calculations within the Kubo formalism

MESOSCOPIC QUANTUM FORMALISM



conditions

 $I_4 = \frac{2e}{\hbar} \sum_{a} I_{4,\alpha}^{spin} = 0$

 $I_1 + I_2 = 0$

Leads free of SOI and disorder

 T_{pq} is the transmission probability of an electron between leads p and q (regardless of spin)

THE TIGHT-BINDING APPROXIMATION



Single band tight-binding model T. P. Pareek and P. Bruno, PRB 63, 165424 (2001) P. Bruno, PRL 79, 4593 (1997)

N x N lattice of constant a_o

Nearest neighbor hopping parameter



Disorder is introduced as local site energy

$$\varepsilon \in \left[-\frac{W}{2}, \frac{W}{2}\right]$$

$$V_R = \frac{\hbar \alpha}{a_0} \qquad V_D = \frac{\hbar \mu}{a_0}$$

THE TIGHT BINDING HAMILTONIAN

$$\begin{split} H &= H_0 + H_R + H_D \\ H_0 &= \sum_{i,\alpha} \varepsilon_i c_{i\alpha}^+ c_{i\alpha} - t \sum_{\langle i,j \rangle \alpha} c_{j\alpha}^+ c_{i\alpha} \\ H_R &= V_R \sum_i \left[\left(c_{i\uparrow}^+ c_{i+\delta_x \downarrow} - c_{i\downarrow}^+ c_{i+\delta_x \uparrow} \right) - i \left(c_{i\uparrow}^+ c_{i+\delta_y \downarrow} - c_{i\downarrow}^+ c_{i+\delta_y \uparrow} \right) \right] \\ H_D &= V_D \sum_i \left[\left(-i \right) \left(c_{i\uparrow}^+ c_{i+\delta_x \downarrow} - c_{i\downarrow}^+ c_{i+\delta_x \uparrow} \right) + \left(c_{i\uparrow}^+ c_{i+\delta_y \downarrow} - c_{i\downarrow}^+ c_{i+\delta_y \uparrow} \right) \right] \end{split}$$

The Hamiltonian incorporates the spin-dependent band structure and the spin-independent disorder.

The SOI causes hopping along the diagonal and is the source of spin-flip scattering

THE RECURSIVE GREEN'S FUNCTION METHOD

$$G = \frac{e^2}{h}T = \frac{e^2}{h} \begin{pmatrix} T^{\uparrow\uparrow} & T^{\uparrow\downarrow} \\ T^{\downarrow\uparrow} & T^{\downarrow\downarrow} \end{pmatrix}$$

$$T_{pq}^{\mu\nu} = Tr \Big[\Gamma_p^{\mu} G_R \Gamma_q^{\nu} G_A \Big]$$

[S. Datta, *Electronic Transport in Mesoscopic Systems*, 1995]

$$\Gamma_p^{\mu} = i \left(\Sigma_p^{\mu} - \Sigma_p^{\mu^+} \right)$$

 Σ_p^{μ} The retarded self-energy function in the isolated lead *p* for spin channel μ

The self energy matrix

$$\Sigma_{p} = \begin{pmatrix} \Sigma_{p}^{\uparrow} & 0 \\ 0 & \Sigma_{p}^{\downarrow} \end{pmatrix}$$
$$G_{R} = \begin{pmatrix} E_{F} - H - \sum_{p=1}^{4} \Sigma_{p} \end{pmatrix}^{-1}$$

$$\Sigma_p^{\uparrow} = \Sigma_p^{\downarrow}$$
 For a perfect metallic lead

LONGITUDINAL AND SPIN HALL CONDUCTANCES

$$\begin{split} T_{pq} &= T_{pq}^{\uparrow\uparrow} + T_{pq}^{\uparrow\downarrow} + T_{pq}^{\downarrow\uparrow} + T_{pq}^{\downarrow\downarrow} \\ T_{pq}^{in} &= T_{pq}^{\uparrow\uparrow} + T_{pq}^{\uparrow\downarrow} - T_{pq}^{\downarrow\uparrow} - T_{pq}^{\downarrow\downarrow} \\ T_{pq}^{out} &= T_{pq}^{\uparrow\uparrow} + T_{pq}^{\downarrow\uparrow} - T_{pq}^{\uparrow\downarrow} - T_{pq}^{\downarrow\downarrow} \end{split}$$

S. Souma and B. K. Nikolic, PRL 94, 106602 (2005)

$$G_{sH} = \frac{I_{3,\uparrow}^{spin} - I_{3,\downarrow}^{spin}}{V_1} = \frac{e}{8\pi} \left(T_{13}^{out} + T_{43}^{out} + T_{23}^{out} - T_{34}^{in} - 2T_{31}^{in} \right)$$
$$G_L = \frac{I_2}{V_1} = \frac{e^2}{h} \left(T_{21} + 0.5T_{32} + 0.5T_{42} \right)$$

G_{sH} Dependence on E_F , V_R , V_D



Clean 20x20 system

For $V_R = V_D$; $G_{sH} = 0$ at any E_F

E_F=-2t

For $V_R/V_D > 1$ and $E_F < 0$ (hole-like), $G_{sH} > 0$, while for $V_R/V_D < 1$, $G_{sH} < 0$

PRB 72, 165335 (2005)

The spin Hall current is generated in the direction of the major driving field.

N. A. Sinitsyn et al., PRB 70, 081312 (2004)B. K. Nikolic et al, PRB 72, 075361 (2005)L. Sheng et al., PRL 94, 016602 (2005)

Typical $a_0=5nm$, m^{*}=0.07m, t =19meV, V_R=1-1.6 meV, V_R/t = 0.05~0.08

G_L AS A FUNCTION OF E_F FOR DIFFERENT DRESSELHAUS COUPLINGS



Longitudinal conductance as a function of V_R and V_D



Spin-Hall conductance as a function of V_R and V_D



 G_{sH} is antisymmetric along the $V_R = V_D$ line

Spin-Hall conductance scaling



 G_{sH} is almost constant up to 50x50, but the boundaries may be important G_{sH} depends on E_F and system size

See also B. K. Nikolic et al., PRB 72, 075361 (2005); L. Sheng et al., PRL 94, 016602 (2005)

\mathbf{G}_{sH} and the effect of disorder





COMPARISON WITH THE KUBO FORMALISM

The general Kubo formulas

$$\sigma_{L}(\vec{r},\vec{r}') = -i\hbar \sum_{n,n'} \frac{f_{n'} - f_{n}}{E_{n'} - E_{n}} \frac{\langle n' | j_{x}(\vec{r}) | n \rangle \langle n | v_{x}(\vec{r}) | n' \rangle}{E_{n'} - E_{n} + i\eta}$$

$$\sigma_{sH}(\vec{r},\vec{r}') = -i\hbar \sum_{n,n'} \frac{f_{n'} - f_{n}}{E_{n'} - E_{n}} \frac{\langle n' | j_{x}^{z}(\vec{r}) | n \rangle \langle n | v_{y}(\vec{r}) | n' \rangle}{E_{n'} - E_{n} + i\eta}$$

$$i\hbar\vec{v} = \left[\vec{r}, H\right]$$
$$j_x^z = \frac{\hbar}{4} \{\sigma_z, v_x\}$$

 $b_n^+ = \sum \psi_n(i,\alpha) c_{i\alpha}^+$

 $i.\alpha$

Single particle states are constructed from the local orbital basis

$$\langle n | \vec{v} | n' \rangle = \frac{1}{i\hbar} \sum_{i,j,\alpha,\beta} \psi_n^*(i,\alpha) [(\vec{r}_i - \vec{r}_j) H_{ij}^{\alpha\beta}] \psi_{n'}(j,\beta)$$

$$\langle n | \vec{j}_z | n' \rangle = \frac{e}{4i} \sum_{i,j,\alpha,\beta} \psi_n^*(i,\alpha) [(\vec{r}_i - \vec{r}_j) \widetilde{H}_{ij}^{\alpha\beta}] \psi_{n'}(j,\beta)$$

$$\widetilde{H} = \{\sigma_z \otimes 1, H\}$$

Comparison of the numerical results with the Kubo formula



Test the effect of the leads The $G_{\rm SH}$ is not a constant, but a function of $\rm E_{\rm F}$ and the SOI coupling

1D AHARONOV-BOHM RING

$$H = \frac{\hbar^2}{2m^*} \left(-i\partial_{\varphi} + \frac{\phi}{\phi_0} \right)^2 + \frac{1}{r} \left[(\alpha \cos \varphi + \beta \sin \varphi) \sigma_x + (\alpha \sin \varphi + \beta \cos \varphi) \sigma_y \left(-i\partial_{\varphi} + \frac{\phi}{\phi_0} \right) - \frac{i}{2r} \left[(\alpha \cos \varphi + \beta \sin \varphi) \sigma_y + (\alpha \sin \varphi + \beta \cos \varphi) \sigma_x \right]$$



Frustaglia and Richter, PRB 69, 235310 (2004) modified to incorporate the Dresselhaus term (CPM&DCM)

$$\phi = \pi r^2 B$$
$$\phi_0 = hc / e$$

J. Phys.:Condens. Mat. 18, 127 (2006)

THE TIGHT BINDING HAMILTONIAN

$$H_{ring} = \sum_{n=1}^{N} \varepsilon_n c_n^+ c_n^- - \sum_{n=1}^{N} \left(t_{n,n+1} c_n^+ c_{n+1}^- + h.c. \right)$$

$$t_{n,n+1}^{0} = te^{(2\pi i/N)(\phi/\phi_{0})}$$

$$t_{n,n+1}^{R} = -it_{R} \left[\cos\frac{\varphi_{n} + \varphi_{n+1}}{2} \sigma_{x} + \sin\frac{\varphi_{n} + \varphi_{n+1}}{2} \sigma_{y} \right]$$

$$t_{n,n+1}^{D} = -it_{D} \left[\sin\frac{\varphi_{n} + \varphi_{n+1}}{2} \sigma_{x} + \cos\frac{\varphi_{n} + \varphi_{n+1}}{2} \sigma_{y} \right]$$



Also in S. Souma and B. K. Nikolic, PRL 94, 106602 (2005) only for Rashba systems

LONGITUDINAL AND SPIN HALL CONDUCTANCE IN A DISORDERED SYSTEM



Averages over 1000 samples

\mathbf{G}_{L} and \mathbf{G}_{sH} AS FUNCTIONS OF THE RASHBA SOI STRENGTH



$$\propto \frac{1}{\sqrt{1+Q_R^2}}$$

G_L IN THE MAGNETIC FIELD



SPIN HALL CONDUCTIVITY IN THE PRESENCE OF THE MAGNETIC FIELD



SPIN ACCUMULATION EFFECTS

Need for time-dependent theory

Nikolic et al, PRL 95, 046601 (2005)

Landauer-Keldysh formalism

$$\left\langle \vec{S}(\vec{r}) \right\rangle = \frac{\hbar}{2} \int_{E_F - eV/2}^{E_F + eV/2} \frac{dE}{2\pi i} Tr_{spin} \left[\hat{\sigma} G^{<}(\vec{r}, \vec{r}; E, V) \right]$$
$$G^{<}(E) = G^{r}(E) \Sigma^{<}(E) G^{a}(E)$$

The non-equilibrium lesser Green's function $G^{<}(E)$ the satisfies the steady state Keldysh equation for quantum transport in a non-interacting system

$$G^{r}(E) = \left[E - H - \Sigma_{L}^{r}(E - eV/2) - \Sigma_{R}^{r}(E + eV/2)\right]^{-1}$$

$$\Sigma^{<}(E) = -2i\left[\operatorname{Im}\Sigma_{L}(E - eV/2) + \operatorname{Im}\Sigma_{R}(E + eV/2)\right]$$

H is the tight binding Hamiltonian



The out-of-plane component $\langle S_{z}(r) \rangle$ of the non-equilibrium spin accumulation

FIG. 1 (color online). (a) The out-of-plane component $\langle S_z(\mathbf{r}) \rangle$ of the nonequilibrium spin accumulation induced by nonlinear quantum transport of unpolarized charge current injected from the left lead into a two-terminal *clean* 2DEG (of size $L = 30a > L_{SO}$, $a \approx 3$ nm) nanostructure with the Rashba SO coupling $t_{SO} = 0.1t_o$ and spin precession length $L_{SO} \approx 15.7a$. (b) Shows how lateral spin- \uparrow and spin- \downarrow densities will *flow* in opposite directions through the attached transverse ideal ($t_{SO} = 0$) leads to generate a linear response spin Hall current $[I_y^s]^z$ out of four-terminal 2DEG ($L = 8a < L_{SO}$) nanostructures [6], which changes sign $[I_y^s]^z(-V) = -[I_y^s]^z(V)$ upon reversing the bias voltage.

Nikolic et al, PRL 95, 046601 (2005)

x is the direction of propagation



FIG. 2 (color online). The one-dimensional transverse spatial profile of the spin accumulation $\langle \mathbf{S}(x = 78a, y) \rangle$ across the $200a \times 200a$ 2DEG with the Rashba SO coupling $t_{\rm SO} = 0.02t_{\rm o}$ through which *ballistic* quantum transport takes place in the nonlinear regime $eV = 0.4t_{\rm o}$ (solid lines) or the linear regime $eV = 10^{-3}t_{\rm o}$ (dotted lines). The width of the edge peaks of $\langle S_z(x = 78a, y) \rangle$ is $\approx L_{\rm SO}/2 = \pi a t_{\rm o}/4t_{\rm SO}$.

EDGE SPIN POLARIZATION EFFECTS

Direct numerical integration of the Schrodinger equation – second order differencing scheme (MSD2) (The leap frog method)

T. litaka, PRB 49, 4684 (1994), Askar, J. Chem. Phys. 68(6), 2794 (1978)

$$i\frac{d}{dt}|\psi,t\rangle = H|\psi,t\rangle$$

$$|\psi,t+\Delta t\rangle = \exp(-iH\Delta t)|\psi,t\rangle$$

MSD2 (second order differencing scheme)

$$|\psi,t+\Delta t\rangle - |\psi,t-\Delta t\rangle = \left[\exp(-iH\Delta t) - \exp(+iH\Delta t)\right]\psi,t\rangle$$

$$\psi(\tau+\Delta \tau) = \psi(\tau-\Delta \tau) - 2iH\Delta \tau \psi(\tau)$$

Scheme is accurate up to $(H\Delta t)^2$

$$\Delta t = 0.01\hbar t^{-1}$$

WAVE PACKET PROPAGATION

Consider a packet propagating along y

$$\psi_{\alpha}(x, y, \tau = 0) = C \sin\left[k_x(x - \overline{x})\right]e^{ik_y(y - \overline{y}) - \frac{(y - \overline{y})^2}{2\sigma^2}}\chi_{\alpha}$$

$$k_x = \frac{n\pi}{a(L+1)}$$
$$\sigma^{-1} = \Delta k_y$$

n-number of open channels

 $E_{F} = 10meV$ $m^{*} = 0.04m$ $k_{y} = 0.35a_{0}^{-1}$ $a_{0} = 3.3nm$ $t \approx 10meV$ $\alpha \approx 50 - 80mVA$ $V_{R} = 1.5 - 2.4meV$

LOCAL SPIN DENSITIES

$S_{x}(i,\tau) = \operatorname{Re}\left\{\psi_{\uparrow}(i,\tau)\psi_{\downarrow}^{*}(i,\tau)\right\}$ $S_{y}(i,\tau) = -i\operatorname{Im}\left\{\psi_{\uparrow}(i,\tau)\psi_{\downarrow}^{*}(i,\tau)\right\}$ $S_{z}(i,\tau) = \left|\psi_{\uparrow}(i,\tau)\right|^{2} - \left|\psi_{\downarrow}^{*}(i,\tau)\right|^{2}$

Contour plots for S_z

(perpendicular on the direction of propagation)

$$V_R = 0.4$$
$$N = 8100$$

n=2



 $\tau_1 = 40\hbar t^{-1}$



$$\tau_2 = 100\hbar t^{-1}$$

S_y

along the direction of propagation





AVERAGE SPIN DENSITIES

y is the direction of propagation !



Averages are done along the longitudinal direction

AVERAGE SPIN ACCUMULATIONS FOR DIFFERENT V_R





Average over 1000 initial disorder configurations

V_R=4.0, N = 8100, n=1

Spin accumulation persists up to W =1.0t

TIME DEPENDENT FORMALISM

The particle source method [T. litaka, Tanaka PRB 57 (1998)]

* Evaluate the matrix elements of the Green's function and those of their products with other quantum operators for large disordered systems *Avoids direct diagonalization of the Hamiltonian when the tight-binding Hamiltonian is used. (CPU time and memory size linear dependent of the system size)

$$i\hbar \frac{d\left|\tilde{j};t\right\rangle}{dt} = H\left|\tilde{j};t\right\rangle + \left|j\right\rangle\theta(t)e^{-i(E+i\eta)t}$$
$$\left|\tilde{j};t=0\right\rangle = 0$$
$$\left|\tilde{j};t\right\rangle = -i\int_{0}^{t} dt' e^{-iH(t-t')}\left|j\right\rangle e^{-i(E+i\eta)t'} = \frac{1}{E+i\eta-H} \left[e^{-i(E+i\eta)t} - e^{-iHt}\right]j\right\rangle$$

For η t>>1, only the first term is relevant

$$\begin{aligned} \left| \tilde{j}; T \right\rangle &\approx \frac{1}{E + i\eta - H} \left| j \right\rangle e^{-i(E + i\eta)T} = G(E + i\eta) \left| j \right\rangle e^{-i(E + i\eta)T} \\ G(E + i\eta) \left| j \right\rangle &= \lim_{T \to \infty} \left| \tilde{j}; T \right\rangle e^{i(E + i\eta)T} \end{aligned} \qquad T = -\frac{\ln \delta}{\eta} \end{aligned}$$

Any state can be chosen as the initial state !

 $\left| j' \right\rangle = AG(E + i\eta) \left| j \right\rangle$

Evaluate the matrix elements of a product including several Green's functions and other operators

The matrix elements of the Green's function can be calculated at many different energy values by solving the equation only once.

$$\begin{split} i\frac{d}{dt}\big|\,\widetilde{j}\,;t\big\rangle &= H\big|\,\widetilde{j}\,;t\big\rangle + \big|\,j\big\rangle \left(\sum_{l} e^{-i(E_{l}+i\eta)t}\right)\theta(t)\\ \big|\,\widetilde{j}\,;t\big\rangle &= -i\int_{0}^{t} dt'\,e^{-iH(t-t')}\big|\,j\big\rangle \left(\sum_{l} e^{-i(E_{l}+i\eta)t'}\right) = \sum_{l} \frac{e^{-i(E_{l}+i\eta)t} - e^{-iHt}}{E_{l} - H + i\eta}\big|\,j\big\rangle\\ \big|\,\widetilde{j}\,;t\big\rangle &\approx \sum_{l} G\big(E_{l} + i\eta\big)\big|\,j\big\rangle e^{-i(E_{l}+i\eta)T} \end{split}$$

$$\frac{1}{T}\int_{0}^{T} dt' \left\langle i \left| \widetilde{j}; t' \right\rangle e^{i(E_{l'}+i\eta)t'} \approx G_{ij} \left(E_{l'}+i\eta \right) \qquad T = \frac{1}{\delta \Delta E}$$

The numerical solution to the Schrodinger equation (leap-frog method)

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

$$\Delta t = \alpha / E_{\max}, \alpha < 1$$

The initial state is a random ket $\left|\Phi\right\rangle = \sum_{n=1}^{N} \left|n\right\rangle e^{i\theta_{n}}$

 $|n\rangle$ are the tight binding orbitals, θ_n are random numbers in [0, 2π]

$$\left\langle e^{i\theta_n}e^{-i\theta_{n'}}\right\rangle_{st}=\delta_{nn'}$$

$$\langle \Phi | A | \Phi \rangle \approx \sum_{n} \langle n | A | n \rangle$$

SPIN ACCUMULATION IN THE BALISTIC REGIME

 $\langle \varsigma \rangle = i \sigma f + f = f \langle n | \sigma | n' \rangle \langle n' | v | n \rangle$

K. Nomura et al., PRB 72, 245330 (2005)



THE KUBO FORMULA Dependence on E_F

$$\sigma_{sH} = \frac{i}{\Omega} Tr \left\{ \delta (E_F - H) j_x^z G_R v_y \right\}$$
$$i\hbar v_y = [y, H]$$
$$j_x^z = \frac{\hbar}{4} \{ \sigma_z, v_x \}$$

Average over 200 initial state vectors and over 100 disordered samples



Nikolic et al., PRB 72, 075361 (2005)

CHARACTERISTIC LENGTH SCALES

Spin procession length

Mean free path (semiclassical expression)



REGIMES

 $L_{S} < L$ semiclassical regime $L_{S} > L$ mesoscopic regime I < L diffusive regimeI > L ballistic regime

L is the system size

$$L_s = \frac{v_F \hbar}{2\alpha k_F}$$

SCALING OF THE SPIN HALL CONDUCTIVITY



The behavior of GsH is strongly correlated with L_s

SCALING OF THE SPIN HALL CONDUCTIVITY (Logarithmic scale)



$$G_{_{sH}} \propto e^{-L/\xi}$$

 $E_{F} = 2.02t$

CONCLUSIONS

Numerical evaluation of the transport parameters in 1D and 2D systems with SOI interaction support the existence of the spin Hall effect as a robust property of the system.