note: Spin Current Simulation in 2D

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To derive the surface Green's function of a semi-infinite chain, we use the fact that an additional site to the chain does not change the physics. From the definition

$$g^r(E) = (E - \mathcal{H} + i\eta)^{-1} \tag{1}$$

where the Hamiltonian $\mathcal{H} = \sum_{\langle ij \rangle}[t_{ij}c_i^\dagger c_j + H.c.]$ is a tight binding model to describe the chain.

1 2D Spin Current

The total dc spin current that is pumped into a two-dimensional system is

$$\left\langle \overline{J_\alpha^z(t)} \right\rangle = \frac{1}{2}\int d\omega \sum_{k\neq 0}[f(\omega+k\Omega)-f(\omega)]\mathrm{Tr}[\boldsymbol{\rho}_\alpha(\omega+k\Omega)\boldsymbol{\gamma}_\alpha \boldsymbol{D}^r_{k;N;N}(\omega')\boldsymbol{\gamma}^\dagger_\alpha(\sigma^z\otimes \boldsymbol{I}_L)\boldsymbol{\rho}_\alpha(\omega)\boldsymbol{\gamma}_\alpha \boldsymbol{D}^a_{-k;N;N}(\omega'+k\Omega)\boldsymbol{\gamma}^\dagger_\alpha] \tag{2}$$

From the expansion of the Green's function in the leading orders of $\Omega_\perp$ for a 1D system, we know

$$D_{1;j,s;j's'}(\omega) = \Omega_\perp \mathcal{G}_{j,s;0\uparrow}(\omega)\mathcal{G}_{0,\downarrow;j's'}(\omega+\Omega) \tag{3}$$

$$D_{-1;j,s;j's'}(\omega) = \Omega_\perp \mathcal{G}_{j,s;0\downarrow}(\omega)\mathcal{G}_{0,\uparrow;j's'}(\omega-\Omega) \tag{4}$$

To derive a similar expression for a 2D system, we notice that the evaluation of Dyson's expansion depends on the perturbative coupling. In a 2D system, we assumed the 0-slice as a series of synchronized precessing magnetization without any interconnection in the zero slice. So the perturbative interaction has a form of

$$\mathcal{H}_1 = \Omega_\perp \left[\sigma^+\delta(\omega'-\omega-\Omega) + \sigma^-\delta(\omega'-\omega+\Omega)\right]\delta_{j0}\delta_{mm'} \tag{5}$$

where the first δ-function assure that the lattice point must be in the zero slice and the second δ-function provide the time dependent interaction to each longitudinal row that is connected to a time-dependent magnetization.

$$\begin{aligned}
\boldsymbol{D}_{1;Njs;Nj's'}(\omega) &= \Omega_\perp \sum_l \mathcal{G}_{Njs;0l\uparrow}(\omega)\,\mathcal{G}_{0l\downarrow;Nj's'}(\omega+\Omega) \\
\boldsymbol{D}_{-1;Njs;Nj's'}(\omega) &= \Omega_\perp \sum_l \mathcal{G}_{Njs;0l\downarrow}(\omega)\,\mathcal{G}_{0l\uparrow;Nj's'}(\omega-\Omega)
\end{aligned} \tag{6}$$

where the matrix representation is

$$\begin{aligned}
\boldsymbol{D}_{1;N;N}(\omega) &= \Omega_\perp\,\boldsymbol{\mathcal{G}}_{N;0}(\omega)\,(\sigma^+\otimes I_M)\,\boldsymbol{\mathcal{G}}_{0;N}(\omega+\Omega) \\
\boldsymbol{D}_{-1;N;N}(\omega) &= \Omega_\perp\,\boldsymbol{\mathcal{G}}_{N;0}(\omega)\,(\sigma^-\otimes I_M)\,\boldsymbol{\mathcal{G}}_{0;N}(\omega-\Omega)
\end{aligned} \tag{7}$$

where M is the dimension of the zero-slice. It is easy to realize that

$$\begin{aligned}
\boldsymbol{D}_{1;N;N}(\omega-\frac{\Omega}{2}) &= \Omega_\perp\,\boldsymbol{\mathcal{G}}_{N;0}(\omega-\frac{\Omega}{2})\,(\sigma^+\otimes I_M)\,\boldsymbol{\mathcal{G}}_{0;N}(\omega+\frac{\Omega}{2}) \\
\boldsymbol{D}_{-1;N;N}(\omega+\frac{\Omega}{2}) &= \Omega_\perp\,\boldsymbol{\mathcal{G}}_{N;0}(\omega+\frac{\Omega}{2})\,(\sigma^-\otimes I_M)\,\boldsymbol{\mathcal{G}}_{0;N}(\omega-\frac{\Omega}{2})
\end{aligned} \tag{8}$$

After substituting into the spin current expression, we find

$$
\begin{aligned}
\langle\overline{J^z_\alpha(t)}\rangle = \frac{\Omega_\perp^2}{2}\int d\omega[f(\omega+\frac{\Omega}{2}) - f(\omega-\frac{\Omega}{2})] \\
\times \Big\{ \mathrm{Tr}\Big[\boldsymbol{\rho}_\alpha(\omega+\frac{\Omega}{2})\,\boldsymbol{\gamma}_\alpha\,\boldsymbol{\mathcal{G}}^r_{N;0}(\omega-\frac{\Omega}{2})\,(\sigma^+\otimes I_M)\,\boldsymbol{\mathcal{G}}^r_{0;N}(\omega+\frac{\Omega}{2})\,\boldsymbol{\gamma}^\dagger_\alpha\,(\sigma^z\otimes I_L) \\
\times\ \boldsymbol{\rho}_\alpha(\omega-\frac{\Omega}{2})\boldsymbol{\gamma}_\alpha\boldsymbol{\mathcal{G}}^a_{N;0}(\omega+\frac{\Omega}{2})(\sigma^-\otimes I_M)\boldsymbol{\mathcal{G}}^a_{0;N}(\omega-\frac{\Omega}{2})\boldsymbol{\gamma}^\dagger_\alpha\Big] \\
-\ \mathrm{Tr}\Big[\boldsymbol{\rho}_\alpha(\omega-\frac{\Omega}{2})\,\boldsymbol{\gamma}_\alpha\,\boldsymbol{\mathcal{G}}^r_{N;0}(\omega+\frac{\Omega}{2})\,(\sigma^+\otimes I_M)\,\boldsymbol{\mathcal{G}}^r_{0;N}(\omega-\frac{\Omega}{2})\,\boldsymbol{\gamma}^\dagger_\alpha\,(\sigma^z\otimes I_L) \\
\times\ \boldsymbol{\rho}_\alpha(\omega+\frac{\Omega}{2})\boldsymbol{\gamma}_\alpha\boldsymbol{\mathcal{G}}^a_{N;0}(\omega-\frac{\Omega}{2})(\sigma^-\otimes I_M)\boldsymbol{\mathcal{G}}^a_{0;N}(\omega+\frac{\Omega}{2})\boldsymbol{\gamma}^\dagger_\alpha\Big]\Big\}
\end{aligned}
\tag{9}
$$

In adiabatic approximation, the spin current can be written as

$$
\begin{aligned}
\langle\overline{J^z_\alpha(t)}\rangle = \frac{\Omega_\perp^2\,\Omega}{2}\int d\omega\,\frac{df}{d\omega} \\
\times \big\{\mathrm{Tr}\big[\boldsymbol{\rho}_\alpha(\omega)\,\boldsymbol{\gamma}_\alpha\,\boldsymbol{\mathcal{G}}^r_{N;0}(\omega)\,(\sigma^+\otimes I_M)\,\boldsymbol{\mathcal{G}}^r_{0;N}(\omega)\,\boldsymbol{\gamma}^\dagger_\alpha\,(\sigma^z\otimes I_L)\,\boldsymbol{\rho}_\alpha(\omega)\,\boldsymbol{\gamma}_\alpha\,\boldsymbol{\mathcal{G}}^a_{N;0}(\omega)\,(\sigma^-\otimes I_M)\,\boldsymbol{\mathcal{G}}^a_{0;N}(\omega)\,\boldsymbol{\gamma}^\dagger_\alpha\big] \\
-\ \mathrm{Tr}\big[\boldsymbol{\rho}_\alpha(\omega)\,\boldsymbol{\gamma}_\alpha\,\boldsymbol{\mathcal{G}}^r_{N;0}(\omega)\,(\sigma^-\otimes I_M)\,\boldsymbol{\mathcal{G}}^r_{0;N}(\omega)\,\boldsymbol{\gamma}^\dagger_\alpha\,(\sigma^z\otimes I_L)\,\boldsymbol{\rho}_\alpha(\omega)\,\boldsymbol{\gamma}_\alpha\,\boldsymbol{\mathcal{G}}^a_{N;0}(\omega)\,(\sigma^+\otimes I_M)\,\boldsymbol{\mathcal{G}}^a_{0;N}(\omega)\,\boldsymbol{\gamma}^\dagger_\alpha\big]\big\}
\end{aligned}
\tag{10}
$$

At zero temperature the derivative of the Fermi distribution turns into a δ-function $\frac{df}{d\omega} = \delta(\omega-\mu)$, where μ is the chemical potential of the reservoir. If we assume that each site in the α slice is connected to a separate reservoir, then $\boldsymbol{\rho}_\alpha = \rho_\alpha \boldsymbol{I}_M$. The current expression can be more simplified to

$$
\begin{aligned}
\langle\overline{J^z_\alpha(t)}\rangle = \frac{\Omega_\perp^2\,\Omega\,t^4}{2}\rho^2_\alpha(\mu)\Big[\mathrm{Tr}\Big\{\boldsymbol{\mathcal{G}}^r_{N;0}(\mu)\,(\sigma^+\otimes I_M)\,\boldsymbol{\mathcal{G}}^r_{0;N}(\mu)\,(\sigma^z\otimes I_L)\,\left[\boldsymbol{\mathcal{G}}^r_{0;N}(\mu)\right]^\dagger\,(\sigma^-\otimes I_M)\,\left[\boldsymbol{\mathcal{G}}^r_{N;0}(\mu)\right]^\dagger\Big\} \\
-\mathrm{Tr}\Big\{\boldsymbol{\mathcal{G}}^r_{N;0}(\mu)\,(\sigma^+\otimes I_M)\,\boldsymbol{\mathcal{G}}^r_{0;N}(\mu)\,(\sigma^z\otimes I_L)\,\left[\boldsymbol{\mathcal{G}}^r_{0;N}(\mu)\right]^\dagger\,(\sigma^-\otimes I_M)\,\left[\boldsymbol{\mathcal{G}}^r_{N;0}(\mu)\right]^\dagger\Big\}\Big]
\end{aligned}
\tag{11}
$$

the sign between two trace must be $+$ instead of $-$.

2 Evaluating Surface Green's Function

To evaluate the surface Green's functions $\boldsymbol{\mathcal{G}}_{0;N}$ and $\boldsymbol{\mathcal{G}}_{N;0}$, we can employ the *Recursive Green's Function* (RGF) technique. We start with the Green's function definition

$$
\mathcal{G}\mathcal{Z} = I \tag{12}
$$

Here we emphasize that $\mathcal{G}$ is the time-independent Green's function of the non-magnetic region. By multiplying the first row of the $\mathcal{G}$ matrix with all columns of the $\mathcal{Z}$ matrix we get set of equations

$$
\mathcal{G}^r_{0;0}(E-\mathcal{H}_0) - \mathcal{G}^r_{0;1}\tau^\dagger = I \tag{13}
$$

$$
-\mathcal{G}^r_{0;0}\tau + \mathcal{G}^r_{01}(E-V_1) - \mathcal{G}^r_{0;2}\tau^\dagger = 0 \tag{14}
$$

$$
\vdots
$$

$$
-\mathcal{G}^r_{0;j-1}\tau + \mathcal{G}^r_{0;j}(E-V_j) - \mathcal{G}^r_{0;j+1}\tau^\dagger = 0 \tag{15}
$$

$$
\vdots
$$

$$
-\mathcal{G}^r_{0;N-2}\tau + \mathcal{G}^r_{0;N-1}(E-V_{N-1}) - \mathcal{G}^r_{0;N}\tau^\dagger = 0 \tag{16}
$$

$$
-\mathcal{G}^r_{0;N-1}\tau + \mathcal{G}^r_{0;N}[E-\gamma^2 g^r_{\alpha\alpha}(\omega)] = 0 \tag{17}
$$

From Eq. (13), we get

$$\mathcal{G}^r_{0;0} = [I + G^r_{0;1}\tau^\dagger]g_0 \tag{18}$$

where $g_0 = (E - \mathcal{H}_0)^{-1}$ is the Green's function of the isolated magnetic slice. After substituting $\mathcal{G}_{0;0}$ into the second equation (14), we get

$$\mathcal{G}^r_{0;1} = [g_0\tau + G^r_{0;2}\tau^\dagger]g_1 \tag{19}$$

where $g_1 = [E - V_1 - \Sigma_0]^{-1}$. Therefore, in general we can write

$$g_j = [E - V_j - \Sigma_{j-1}]^{-1}, \qquad \Sigma_{j-1} = \tau^\dagger g_{j-1}\tau \tag{20}$$

and

$$\mathcal{G}^r_{0;j} = [g_0\,\tau\,g_1\,\tau\,\ldots\,g_{j-1}\,\tau + \mathcal{G}_{0;j+1}\tau^\dagger]g_j \tag{21}$$

Finally, after sweeping over whole NM region from left to right, we get the surface Green's function $\mathcal{G}^r_{0N}$

$$\mathcal{G}^r_{0N} = g_0\,\tau\,g_1\,\tau\,\ldots\,g_{N-1}\,\tau\,g_N \tag{22}$$

where

$$g_N = [E - \gamma^2 g^r_{\alpha\alpha} - \Sigma_{N-1}]^{-1} \tag{23}$$

The same procedure can be followed to arrive a recursive algorithm to evaluate $\mathcal{G}^r_{N;0}$. In summary

$$\mathcal{G}^r_{N;0} = g_N\,\tau^\dagger\,g_{N-1}\,\tau^\dagger\,\ldots\,g_2\,\tau^\dagger\,g_1\,\tau^\dagger\,g_0 \tag{24}$$

where

$$g_j = [E - V_j - \Sigma_{j+1}]^{-1}, \qquad \Sigma_{j+1} = \tau g_{j+1}\tau^\dagger \tag{25}$$

except

$$g_N = [E - \gamma^2 g^r_{\alpha\alpha}]^{-1}, \qquad g_0 = [E - \mathcal{H}^0 - \Sigma_1]^{-1} \tag{26}$$

Few questions need careful attention:

- In this algorithm, we start from the magnetic site, to evaluate the retarded Green's function, an infinitesimal imaginary number must be added to the Hamiltonian, however, if one start the calculation from the slice α then the imaginary part in inherited from the reservoir. Do these two approach are equivalent? (notice that in the second approach two sweeps are needed.

- Is it possible to evaluate both $\mathcal{G}_{0;N}$ and $\mathcal{G}_{N;0}$ with one sweep? Does an inversion symmetry help for faster evaluation? Consider inversion operator $\boldsymbol{I}$ where the system remains invariant under inversion $\boldsymbol{I}\mathcal{Z} = \mathcal{Z}$.

To evaluate $\mathcal{G}_{N;0}$, we derive a set of equations by multiplying the last row of $\mathcal{G}$ by $\mathcal{Z}$ matrix

$$\mathcal{G}^r_{N;0}(E - \mathcal{H}_0) - G^r_{N;1}\tau^\dagger = 0 \tag{27}$$

$$-\mathcal{G}^r_{N;0}\tau + \mathcal{G}^r_{N;1}(E - V_1) - G^r_{N;2}\tau^\dagger = 0 \tag{28}$$

$$\vdots$$

$$\mathcal{G}^r_{N;j-1}\tau + \mathcal{G}^r_{N;j}(E - V_j) - \mathcal{G}^r_{N;j+1}\tau^\dagger = 0 \tag{29}$$

$$\vdots$$

$$-\mathcal{G}^r_{N;N-1}\tau + \mathcal{G}^r_{N;N}[E - \gamma^2 g^r_{\alpha\alpha}] = I \tag{30}$$

In the same manner we start from Eq. (27), we write

$$\mathcal{G}^r_{N;N} = [I + \mathcal{G}^r_{N;N-1}\,\tau]g_N, \qquad g_N = [E - \gamma^2 g^r_{\alpha\alpha}]^{-1} \tag{31}$$

The general expression will be

$$G^r_{N;j} = [I + G^r_{N;j-1}\tau]g_j, \qquad g_j = [E - V_j - \Sigma_{j-1}]^{-1} \tag{32}$$

3 Spin-Orbit Interaction in Tight-Binding Model

To give an expression for the SOI in the tight-binding model we start with Dresselhaus SOI, with intrinsic source of electric potential in the plane of a 2D system:

$$\begin{aligned}
\mathcal{H}_{\mathrm{D}} &= \frac{1}{2m}(\mathbf{p}-e\mathbf{A})^2 - \boldsymbol{\mu}\cdot\mathbf{B} \\
&= \frac{1}{2m}(\mathbf{p}-e\mathbf{A})^2 - \alpha\boldsymbol{\sigma}\cdot[(\mathbf{p}-e\mathbf{A})\times\boldsymbol{\nabla}V] \\
&= \frac{1}{2m}(\mathbf{p}-e\mathbf{A})^2 - \alpha\boldsymbol{\sigma}\cdot[(\frac{\hbar}{i}\partial_x - eA_x)\partial_y V - (\frac{\hbar}{i}\partial_y - eA_y)\partial_x V]
\end{aligned} \tag{33}$$

where can be discretized into a form of

$$\begin{aligned}
\mathcal{H}_{\mathrm{D}} = \frac{\lambda\hbar}{2a}\sum_{n,m}\{&[\partial_x V]_{n,m\to m+1}(|n,m\rangle\langle n,m+1|\otimes i\sigma^z) \\
&[\partial_y V]_{n\to n+1,m}e^{-i2\pi\sum_{l<m}\frac{\Phi_{n,l}}{\Phi_0}}(|n,m\rangle\langle n+1,m|\otimes i\sigma^z) + \text{H.C}\Big\}
\end{aligned} \tag{34}$$

On the other hand, the Rashba SOI with a source of electric filed due to broken symmetry in z-direction, can be written in the form of

$$\begin{aligned}
\mathcal{H}_{\mathrm{R}} &= \frac{1}{2m}(\mathbf{p}-e\mathbf{A})^2 - \alpha(\sigma\times\mathbf{p})\cdot\mathbf{E} \\
&= \frac{1}{2m}(\mathbf{p}-e\mathbf{A})^2 - \alpha(\sigma\times\frac{\hbar}{i}\boldsymbol{\nabla})_z E_0 \\
&= \frac{1}{2m}(\mathbf{p}-e\mathbf{A})^2 + i\alpha(\sigma_x\partial_y - \sigma_y\partial_x).
\end{aligned} \tag{35}$$

The discrete form for the tight-binding model will be

$$\mathcal{H}_{\mathrm{R}} = -t_{so}\sum_{n,m}\left\{e^{-i2\pi\sum_{l<m}\frac{\Phi_{n,l}}{\phi_0}}(|n,m\rangle\langle n+1,m|\otimes i\sigma^y) - (|n,m\rangle\langle n,m+1|\otimes i\sigma^x) + \text{H.C.}\right\} \tag{36}$$

4 Analytical Evaluation of the Spin Currents in a 2D Square Lattice

A minimal system to evaluate the spin current in a 1D chain consists of one site sandewiched between the reservoir and the magnetic site. From the definition of the Green's function, we have

$$\begin{pmatrix} G_{00} & G_{01} \\ G_{10} & G_{11} \end{pmatrix}\begin{pmatrix} E-\Omega_\parallel\sigma_z & -t_x \\ -t_x & E-\gamma_\alpha^2 g_{\alpha\alpha}(E) \end{pmatrix} = \boldsymbol{I} \tag{37}$$

To find G_{01}, we multiply the first row of the Green's function's matrix with the Hamiltonian to derive the set of equations

$$\begin{aligned}
G_{00}(E-\Omega_\parallel\sigma_z) - G_{01}t_x &= 1 \\
-G_{00}t_x + G_{01}(E-\gamma_\alpha^2 g_{\alpha\alpha}(E)) &= 0
\end{aligned} \tag{38}$$

From the first equation, we find

$$G_{00} = (1+G_{01}t_x)g_M \tag{39}$$

where $g_M = (E-\Omega_\parallel\sigma_z)^{-1}$ is the Green's function of the decoupled magnetic site. After substituting into the second equation, we get

$$G_{01} = -g_M t_x[E-\gamma_\alpha^2 g_{\alpha\alpha}(E) - t_x g_M]^{-1} \tag{40}$$

In a 1D chain, the Green's function of a semi-finite reservoir is $g_{\alpha\alpha}(E) = \frac{e^{-i\phi_v}}{t_x}$ and the Green's function of the isolated magnetic site

$$g_M = \begin{pmatrix} E - \Omega_\parallel & 0 \\ 0 & E + \Omega_\parallel \end{pmatrix}^{-1} = \begin{pmatrix} \frac{1}{E-\Omega_\parallel} & 0 \\ 0 & \frac{1}{E+\Omega_\parallel} \end{pmatrix} \tag{41}$$

From this, we can evaluate G_{01} using Eq. (37) to find

$$G_{01} = -t_x \begin{pmatrix} \frac{1}{E-\Omega_\parallel} & 0 \\ 0 & \frac{1}{E+\Omega_\parallel} \end{pmatrix} \begin{pmatrix} E - \gamma_\alpha^2 \frac{e^{-i\phi_v}}{t_x} - \frac{t_x}{E-\Omega_\parallel} & 0 \\ 0 & E - \gamma_\alpha^2 \frac{e^{-i\phi_v}}{t_x} - \frac{t_x}{E+\Omega_\parallel} \end{pmatrix}^{-1} \tag{42}$$

$$= \begin{pmatrix} \frac{t_x}{(Et_x - \gamma_{\alpha\alpha}^2 e^{-i\phi_v})(E-\Omega_\parallel) - t_x^2} & 0 \\ 0 & \frac{t_x}{(Et_x - \gamma_{\alpha\alpha}^2 e^{-i\phi_v})(E+\Omega_\parallel) - t_x^2} \end{pmatrix} \tag{43}$$

In the same way, two different approaches can be employed to evalute G_{10}. The set of equation that we derived by multiplying the Green's function with the Hamiltonian are

$$G_{10}(E - \Omega_\parallel \sigma_z) - t_x G_{11} = 0 \tag{44}$$

$$-t_x G_{10} + G_{11}[E - \gamma_\alpha^2 g_{\alpha\alpha}(E)] = 1 \tag{45}$$

4.1 Approach I

From the second equation we can write

$$G_{11} = (1 + t_x G_{10}) g_R \tag{46}$$

where g_R is the Green's function of the decoupled reservoir $g_R = [E - \gamma_\alpha^2 g_{\alpha\alpha}(E)]^{-1}$. After substituting G_{11} into the first equation, we find

$$G_{10}(E - \Omega_\parallel \sigma_z) - t_x g_R - t_x^2 G_{10} g_R = 0 \tag{47}$$

to finally get

$$G_{10} = t_x g_R [E - \Omega_\parallel \sigma_z - t_x^2 g_R]^{-1} \tag{48}$$

4.2 Approach II

We can find G_{11} from the first equation $G_{10}(E - \Omega_\parallel \sigma_z) = t_x G_{11}$ and substitute into the second one to get

$$-t_x G_{10} + \frac{G_{10}}{t_x}(E - \Omega_\parallel \sigma_z)[E - \gamma_{\alpha\alpha}^2 g_{\alpha\alpha}(E)] = 1 \tag{49}$$

and finally we get

$$G_{10} = t_x \left[(E - \Omega_\parallel \sigma_z)(E - \gamma_\alpha^2 g_{\alpha\alpha}) - t_x^2\right]^{-1} = t_x \left[g_M^{-1} g_R^{-1} - t_x^2\right]^{-1} \tag{50}$$

From the first approach relation we find

$$G_{10} = \begin{pmatrix} e^{-i\phi_v} & 0 \\ 0 & e^{-i\phi_v} \end{pmatrix} \begin{pmatrix} E - \Omega_\parallel - t_x^2 g_R & 0 \\ 0 & E + \Omega_\parallel - t_x^2 g_R \end{pmatrix}^{-1} \tag{51}$$

$$= \begin{pmatrix} \frac{e^{-i\phi_v}}{E-\Omega_\parallel - t_x^2 g_R} & 0 \\ 0 & \frac{e^{-i\phi_v}}{E+\Omega_\parallel - t_x^2 g_R} \end{pmatrix} \tag{52}$$

It is easy to show that both approaches leads to the same result.