Spin-inelastic scattering in two-dimensional systems with Rashba spin-orbit coupling

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We consider spin-inelastic scattering off magnetic impurity in a spin chiral two-dimensional electron gas, e.g. Rashba system, and the emergence of inelastic Friedel oscillations. Spin-inelastic contributions generate strong charge redistribution which will be detectable in the tunneling conductance only at specific bias voltages corresponding to the energy of the inelastic mode.

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Measurements of inelastic transitions open up a route to investigate the excitation spectrum of physical systems. There has been a growing activity in elucidating inelastic scattering processes in quantum systems using various experimental techniques. An incomplete list includes inelastic neutron$^{1,2}$ and X-ray$^{3,4}$ scattering, transport through break junctions,$^{5,6}$ and scanning tunneling microscopy (STM) with spin-polarized (SP-STM)$^{7,8}$ or non spin-polarized tip.$^{9−17}$

Surface imaging of scattering states can be performed e.g. by using STM to probe the spatial spectral density variations at a given energy. It is well-known that Friedel oscillations emerge around defects adsorbed onto a surface caused by elastic scattering processes.$^{18,19}$

Less known is the prediction made earlier that points to the existence of inelastic Friedel oscillations emerging from vibrating impurities.$^{20−22}$ These oscillations were recently demonstrated experimentally for dimers of meta-dichlorobenzene.$^{23}$ The mechanism for inelastic Friedel oscillations is essentially the same as for conventional oscillations and comes from interference of incoming and outgoing waves that have an energy mismatch given by energy transferred to incoming and outgoing waves that have an energy mismatch given by energy transferred to the external magnetic field

\[ B \]

or non spin-polarized tip.$^{9−17}$

A major difference in the present set-up compared to the ones considered in e.g., Ref. 24, is that the Rashba surface is magnetically active in the sense that a magnetic contrast emerges around the adsorbed local impurities. This contrast can be probed using a SP-STM set-up where the scanning tip has a finite component of the magnetic moment parallel to the surface plane.

In order to provide a concrete example of the effect we propose, consider a collection of general spins $S_n(t) = S(r_n,t)$ located at the positions $r_n$ on a spin chiral metallic substrate surface. In terms of the spinor $\Psi_k = (c_{k\uparrow} c_{k\downarrow})^T$, the surface electron density can be modeled by

\[ H_{\text{surf}} = \sum_k \Psi_k^\dagger \hat{c}_k \sigma^0 + \alpha (k \times \hat{z}) \cdot \sigma \Psi_k, \]  

(1)

where $\hat{c}_k$ denotes the single electron energy at the momentum $k$ and $\alpha$ defines the Rashba spin-orbit coupling. Here, $\sigma^0$ is the $2 \times 2$ identity matrix and $\sigma$ is the vector of Pauli matrices. The interaction between the localized magnetic moments and the surface states is captured within the Kondo interaction model

\[ H_K = \nu_u \sum_n s(r_n,t) \cdot S_n(t), \]  

(2)

where $\nu_u$ is the unit area and $J_K$ is the Kondo exchange parameter.

The electron spin is denoted by $s(r_n,t) = \Psi(t) \sigma \Psi(t)$ while $\Psi(t) = \sum_k \Psi_k(t)e^{ikr}$. We include the external magnetic field $B$ acting on the spin and on the surface electrons, i.e.

\[ H_{\text{ext}} = -g \mu_B B \cdot S_n(t) - g \mu_B |B| \sum_k \Psi_k^\dagger \sigma^z \Psi_k / 2, \]  

(3)

where $g$ and $\mu_B$ are the gyromagnetic ratio and Bohr magneton, respectively.

In our calculated examples below, we assume that the localized spin moments can be described in terms of the Hamiltonian

\[ H_S = \sum_n \{D(S_n^z)^2 + E[(S_n^x)^2 + (S_n^y)^2] / 2 \} \]  

(4)

where the anisotropy fields $D$ and $E$ account for the effective interaction between the localized spin moments and the surface electrons. In terms of this model, we define
the $2S + 1$ eigenstates $|\alpha\rangle$ and corresponding eigenenergies $E_{\alpha}$, where $\alpha \in \{-S, -S + 1, \ldots, S\}$.

We account for scattering off the magnetic impurities by calculating the real space Green function (GF) for the surface electrons using $G(r, r'; \omega) = \frac{1}{2\pi i} \int G(k, k'; \omega) e^{ikr - ik'r'} dkdk'/(2\pi)^4$, where $G(k, k'; \omega) = \langle \sigma \sigma' | \langle \mathbf{k} | \mathbf{k}' \rangle_{\omega} \rangle$ is a $2 \times 2$ matrix, with spin indices $\sigma, \sigma' = \uparrow, \downarrow$.

First we construct a bare GF $G^{(0)}$ which contains the spin-polarization induced by the localized magnetic moments. In the model of the substrate, i.e. $H_{\text{surf}} + H_K$, we obtain the matrix (spin space) equation

$$G^{(0)}(\mathbf{k}, \mathbf{k'}) = \delta(\mathbf{k} - \mathbf{k'}) g(\mathbf{k}) + \int g(\mathbf{k}) V_\nu e^{-(ik-p)\tau} G^{(0)}(\mathbf{p}, \mathbf{k'}) \frac{dp}{(2\pi)^2}$$

where $V_\nu = V_0 + \sigma \cdot \Delta_\nu(\omega)$ is the scattering potential comprising the spin-independent and spin-dependent contributions $V_0$ and $\Delta_\nu(\omega) = v_0 k \langle S_\nu(\omega) \rangle$, respectively, whereas $g(\mathbf{k})$ is the GF for the free surface states. In spirit of scattering theory, we obtain a T-matrix formulation of the first order GF, by expanding Eq. (5), giving

$$G^{(0)}(\mathbf{k}, \mathbf{k'}) = \delta(\mathbf{k} - \mathbf{k'}) g(\mathbf{k}) + g(\mathbf{k}) e^{-ik' \mathbf{r}_m} T(\mathbf{r}_m, \mathbf{r}_m) g(\mathbf{k'}) e^{ik' \mathbf{r}_m},$$

where $T(\mathbf{r}_m, \mathbf{r}_m) = t(\mathbf{r}_m, \mathbf{r}_m) V_{\mathbf{m}_\nu}$

We connect our results for the local DOS to the differential conductance $\frac{dI}{dV}$ of the STM measurements through the formula

$$\frac{dI}{dV} \propto n_0 N(\mathbf{r}, V) + m_0 \cdot \mathbf{M}(\mathbf{r}, V),$$

where $n_0$ and $m_0$ is the DOS and magnetization of the tip whereas $N(\mathbf{r}, V) = -Tr\mathbf{M}(\mathbf{r}, V) \tau$ and $\mathbf{M}(\mathbf{r}, V) = -Tr\mathbf{M}(\mathbf{r}, V) \tau$ are the corresponding quantities of the surface at the spatial position $\mathbf{r}$ and voltage bias $V$.

### A. Single impurity

The GF for the free surface electrons is given by

$$g(\mathbf{k}, \omega) = \frac{(i\omega - \varepsilon_k)\alpha_0 + \alpha \mathbf{k} \cdot \mathbf{z}}{(i\omega - \varepsilon_k)^2 - \alpha^2 k^2},$$

where $k = |\mathbf{k}|$. The corresponding retarded real space GF is given by

$$g^r(\mathbf{r}, \omega) = \frac{1}{N_0} \sum_{k = \pm} t_{1/2}^{(\mathbf{r})}(\kappa, \mathbf{r}) \kappa_\nu,$$

$$g_0(\mathbf{r}, \omega) = -\frac{1}{N_0} \sum_{k = \pm} t_{1/2}^{(\mathbf{r})}(\kappa, \mathbf{r}) \kappa_\nu \mathbf{r} \cdot \mathbf{z},$$

with $\kappa = \sqrt{2N_0(\omega + \alpha^2 N_0/2)}$, $\kappa_\nu = \kappa \pm \alpha N_0$, $N_0 = m/\hbar^2$, and $\mathbf{r} = \mathbf{r}/|\mathbf{r}|$. Here also, $H^{(1)}_{\mathbf{r}}(z)$ is the Hankel function. The magnetic structure of the free surface states can be written $m(\mathbf{r}, \omega) = -Tr \mathbf{M}(\mathbf{r}, \omega)/\pi = (m_{1}(\mathbf{r}, \omega), m_{2}(\mathbf{r}, \omega))$ with vanishing spin-polarization $m_{2}(\mathbf{r}, \omega) = 0$. There is, nonetheless, an in-plane magnetic structure $m_{1}(\mathbf{r}, \omega) = -Tr\mathbf{M}(\mathbf{r}, \omega)/\pi$.

The bare GF $G^{(0)}$ is defined from the T-matrix expansion

$$G^{(0)}(\mathbf{k}, \mathbf{k'}) = \delta(\mathbf{k} - \mathbf{k'}) g(\mathbf{k}) + e^{-i\mathbf{k} \cdot \mathbf{r}} g(\mathbf{k}) T g(\mathbf{k'}) e^{i\mathbf{k'} \cdot \mathbf{r}},$$

and

$$T = \left( V^{-1} - g(\mathbf{r} = 0) \right)^{-1} = \frac{T_0}{\alpha^2 + \Delta^2 / t_0},$$

$$T_0 = V_0 + i(V_0^2 - |\Delta|^2) N_0/2,$$

since $g(\mathbf{r} = 0) = \int g(\mathbf{k}) dk/(2\pi)^2 = -iN_0/2$. The correction $\delta G^{(0)}(\mathbf{k}, \mathbf{k'}) = e^{-i\mathbf{k} \cdot \mathbf{r}} g(\mathbf{k}) T g(\mathbf{k'}) e^{i\mathbf{k'} \cdot \mathbf{r}}$ is partitioned into charge and magnetic contributions $\delta G^{(0)}(\mathbf{k}, \mathbf{k'}) = \delta g_0(\mathbf{k}, \mathbf{k'}) \alpha_0 + \delta g_1(\mathbf{k}, \mathbf{k'}) \cdot \mathbf{r}$, where

$$\delta g_0(\mathbf{k}, \mathbf{k'}) = t_0^{-1} \left( g_0(\mathbf{k}) T_0 + g_1(\mathbf{\Delta}) g_0(\mathbf{k'}) \right)$$

and

$$\delta g_1(\mathbf{k}, \mathbf{k'}) = t_0^{-1} \left( g_0(\mathbf{k}) T_0 + g_1(\mathbf{\Delta}) g_0(\mathbf{k'}) \right) + i\nu\left( g_0(\mathbf{k}) T_0 + i g_1(\mathbf{\Delta}) \right) \times g_0(\mathbf{k'}).$$

By the same token we write the real space GF

$$G^{(0)}(\mathbf{r}, \mathbf{r'}) = g(\mathbf{r} - \mathbf{r'}) + \delta G^{(0)}(\mathbf{r}, \mathbf{r'})$$

where the correction term $\delta G^{(0)}(\mathbf{r}, \mathbf{r'}) = g(\mathbf{r} - \mathbf{r}) T g(\mathbf{r}) - g(\mathbf{r} - \mathbf{r'}) = \delta g_0(\mathbf{r}, \mathbf{r'}) \alpha_0 + \delta g_1(\mathbf{r}, \mathbf{r'}) \cdot \mathbf{r}$. The components $\delta g_0(\mathbf{r}, \mathbf{r'})$ and $\delta g_1(\mathbf{r}, \mathbf{r'})$ are given by Eq. (11) by replacing $\mathbf{k} \rightarrow \mathbf{r} = \mathbf{r} - \mathbf{r}_0$ and $\mathbf{k'} \rightarrow -\mathbf{R}_0 = \mathbf{r}_0 + \mathbf{r'}$. We find the correction to the density of electron states (DOS) $\delta N(\mathbf{r}, \omega)$ and magnetic structure $\delta \mathbf{M}(\mathbf{r}, \omega)$ respectively given by

$$\delta N^{(0)}(\mathbf{r}, \omega) = -\frac{1}{\pi t_0} \left( g_0^2(\mathbf{R}_0) + g_0^2(\mathbf{R}_0) \right)$$

and

$$\delta \mathbf{M}^{(0)}(\mathbf{r}, \omega) = -\frac{1}{\pi t_0} \left( g_0^2(\mathbf{R}_0) - g_0^2(\mathbf{R}_0) \right) \mathbf{A}$$
FIG. 1: Calculated differential conductance $dI(t)/dV$ around an adsorbed spin moment for increasing (left to right) Rashba coupling strength parameter $a = a_0(1/10, 1, 10)$, where $a_0 = 0.1253$ Å. Other parameters are effective electron mass $m' = 0.38m_e$, with free electron mass $m_e$, temperature $T = 0.1$ K, quadratic energy dispersion for the surface states $E_{surf}(k) = E_F = E_0 + k^2/2N_0$, with $E_0 = -0.45$ eV. The tip is assumed to have a magnetic moment $m_{tip} = 3n_0(1,0,0)$, where $n_0$ is the tip DOS at the Fermi level.

In Fig. 1 we plot the calculated differential conductance $dI(t)/dV$ for different strengths of the Rashba coupling parameter $a$, assuming a STM tip with finite magnetic moment $m_0$ parallel to the surface plane. The local defect has a clear impact on the electronic structure in all three cases, as expected. However, only for sufficiently strong Rashba coupling the magnetic structure is significantly modified, panels (b) and (c), to generate a magnetic contrast, or asymmetry around the defect, in the resulting differential conductance.

In second order perturbation theory with respect to $v_0f_k$, effects from spin-inelastic scattering off the localized spin moments influences the surface state. We define the self-energy

$$\Sigma_{a\sigma'}(r_n, m_n; i\omega) = -\frac{(v_0f_k)^2}{\beta} \sum_{\sigma} \sigma_{a\sigma'} \chi_{a\sigma}(iv) \cdot \sigma_{a\sigma'} \times G^{(0)}_{a\sigma}(r_n, m_n; i\omega - iv)$$

(14)

The factor $\beta^{-1} = k_B T$ where the spin-spin GF $\chi_{a\sigma}(iv)$ is the Fourier transform of $\chi_{a\sigma}(t, t') = (i)\langle TS_{a}(t)S_{a}(t')\rangle$. In real space, we have the GF expansion

$$G(r, r') = G^{(0)}(r, r') + \sum_{nm} G^{(0)}(r, m) \Sigma(r_n, m_n) G^{(0)}(m, r').$$

(15)

For the spin-spin GF we make the approximation $\chi_{a\sigma}(t, t') \approx (i)\langle T\sigma G_{mn}(t, t')\rangle$ as we focus on the main effect due to spin-inelastic scattering. Here, $G_{mn} = [G_{a\sigma\beta\gamma}]$ is the single electron GF defined on the spin states $|a\rangle$ over which the trace runs. Assuming that the basis $|a\rangle$ is an eigenbasis the GF $G_{mn}$ becomes diagonal, such that we can write $G_{mn} = \delta_{mn} G_{a\beta\gamma}$. The correction term $\delta G = G^{(0)} \Sigma G^{(0)}$ in Eq. (15) then acquires the form

$$\delta G(r, r; i\omega) = \sum_{nm} G^{(0)}(r, m; i\omega) \int L(i\omega; \epsilon) \times \text{Im}G^{(0)}(r, m; \epsilon) \frac{d\epsilon}{\pi} = G^{(0)}(r, r; i\omega),$$

(16a)

$$L(i\omega; \epsilon) = (v_0f_k)^2 \sum_{a\beta} \tau_{a\beta}(i\omega + \tau_{a\beta} - \tau_{a\beta}) + \tau_{a\beta} \times \tau_{a\beta} \cdot \sigma$$

$$\times \frac{f(E_a)f(-E_b) - f(E_a)f(-E_b)f(\epsilon)}{i\omega - E_a + E_b + \epsilon}. \ (16b)$$

The factor $L$ clearly indicates that the correction term $\delta G$ become active for energies near the transition energy $\Delta_{a\beta} = E_a - E_b$, such that processes corresponding to both emission and absorption of the energy quanta $\Delta_{a\beta}$ are accounted for. Moreover, processes that correspond to both spin conserving and spin non-conserving of the local spin moment are included by the products $\tau_{a\beta} \times \tau_{a\beta}$ and $\tau_{a\beta} \times \tau_{a\beta}$, respectively. The former processes will be stimulated when the electrons either emit or absorb the appropriate energy quantum to the spin system while no change in spin (angular) momentum is required, that is, transitions between spin states with the same spin projection $m$. The latter processes, on the other hand, correspond to transitions between states with different spin projections differing by a total spin moment of one (1). Those will be stimulated by electrons that deposit or absorb the appropriate energy quantum accompanied by a spin flip.

As done above, we partition the correction into charge and magnetic components according to $\delta G = \delta G_{00} + \delta G_{1\sigma}$, see Appendix A. It is clear that the factor $L$ influences both the DOS and magnetic structure. The variations in the DOS can be captured by non spin-polarized STM and, particularly, in the inelastic electron tunneling spectroscopy (IETS) $dI/dV^2$. Variations in the magnetic structure, however, has to be probed using SP-STM.

In Fig. 2 we summarize those observations for a single impurity calculated for under the same conditions as in Fig. 1. The differential conductance (bold) displays the increased differential conductance at the spin-inelastic transitions (16 and 24 meV), given a spin $S = 1$ impurity and anisotropy fields $D = -2$ meV and $E = |D|/5$. The differential conductance far off the spin impurity is plotted (faint) for reference. The IETS shown in panel (b) shows peaks and dips at spin-inelastic transitions, and the spectrum suggests that one can generate IETS maps, panel (c), at different energies with varying contrast depending on whether the probe voltage corresponds to the spin-inelastic transitions or not.

We have studied the influence of local magnetic moment on the surface states with Rashba spin orbit coupling. The elastic scattering generates Friedel oscillations around the impurity due to charge redistribution caused by the presence of the impurity. For strong enough Rashba coupling parameter, the magnetic structure surrounding the impurity becomes significantly dis-
FIG. 2: Calculated (a) differential conductance \( dI/dV \), (b) IETS \( d^2I(r,V)/dV^2 \) at \( r - r_0 = (0,2) \) Å and (c) IETS maps at the voltages \( V = -3.5, -2.1, -1.7, -1.4, -1.0 \) mV, for Rashba coupling strength parameter \( \alpha = \alpha_0 \), around a single \( S = 1 \) impurity with anisotropy fields \( D = \pm 2 \) meV and \( E = |D|/5 \). The positions of the bare absorption peaks (16 and 24 meV) are signified by bars in panel (b). Other parameters are as in Fig. 1.

The positions of the bare absorption peaks (16 and 24 meV) are signified by bars in panel (b). Other parameters are as in Fig. 1.

Torst when probed using SP-STM, where the tip magnetic moment has a finite component parallel to the surface plane.

We have, further, shown that inelastic spin transitions will generate changes in the differential conductance as the inelastic scattering open additional channels for conduction. At the onset of those channels, the IETS \( (d^2I/dV^2) \) display peaks/dips. The local electronic structure surrounding the impurity becomes distorted at voltages corresponding to the spin-inelastic transitions, so-called inelastic Friedel oscillations. A sufficiently strong Rashba coupling gives rise to significant changes in the magnetic structure at voltages near the spin-inelastic transitions.

In view of recent observations of single Fe atoms adsorbed on Ptn(111)\(^{16}\) and Co atoms on graphene,\(^{17}\) we believe that our predictions for magnetic defects on metallic chiral surfaces will be verifiable.

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Appendix A: Correction term

\[ \delta G_0(r, r') = \frac{1}{\pi} \int L(i\omega; \epsilon) \left( (G_0^{(0)}(r, r_n) \text{Im}G_0^{(0)}(r_n, r_m) + G_1^{(0)}(r, r_n) \cdot \text{Im}G_1^{(0)}(r_n, r_m))G_0^{(0)}(r_m, r') ight. \\
+ (G_0^{(0)}(r, r_n) \text{Im}G_1^{(0)}(r_n, r_m) + G_1^{(0)}(r, r_n) \cdot \text{Im}G_0^{(0)}(r_n, r_m) + iG_1^{(0)}(r, r_n) \times \text{Im}G_1^{(0)}(r_n, r_m)) \cdot G_1^{(0)}(r_m, r') d\epsilon, \quad (A1a) \]

\[ \delta G_1(r, r') = \frac{1}{\pi} \int L(i\omega; \epsilon) \left( (G_0^{(0)}(r, r_n) \text{Im}G_0^{(0)}(r_n, r_m) + G_1^{(0)}(r, r_n) \cdot \text{Im}G_1^{(0)}(r_n, r_m))G_1^{(0)}(r_m, r') ight. \\
+ (G_0^{(0)}(r, r_n) \text{Im}G_1^{(0)}(r_n, r_m) + G_1^{(0)}(r, r_n) \cdot \text{Im}G_0^{(0)}(r_n, r_m) + iG_1^{(0)}(r, r_n) \times \text{Im}G_1^{(0)}(r_n, r_m))G_1^{(0)}(r_m, r') \\
+ \left. i(G_0^{(0)}(r, r_n) \text{Im}G_1^{(0)}(r_n, r_m) + G_1^{(0)}(r, r_n) \cdot \text{Im}G_0^{(0)}(r_n, r_m) + iG_1^{(0)}(r, r_n) \times \text{Im}G_1^{(0)}(r_n, r_m)) \times G_1^{(0)}(r_m, r') d\epsilon. \quad (A1b) \]