Kinetic theory with spin−orbit coupling in magnetic fields

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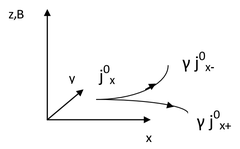
MAX-PLANCK-GESELLSCHAFT

Phenomenological considerations

charge current density $\mathbf{j}_n^0 = -\mu n\mathbf{E} - D\nabla n$
spin polarization current density $S_{ij}^0 = -\mu E_i s_j - D\frac{\partial s_j}{\partial x_i}$
with mobility μ, diffusion D and spin polarization density $s_z = (n_\uparrow - n_\downarrow)/2$



$$j_y^{\rm s.o.} = j_{+y}^{\rm s.o.} + j_{-y}^{\rm s.o.} = \gamma\mu(n_+ - n_-)E_x + \gamma D\frac{\partial(n_+ - n_-)}{\partial x}$$
$$S_{yz}^{\rm s.o.} = j_{+y}^{\rm s.o.} - j_{-y}^{\rm s.o.} = \gamma\mu(n_+ + n_-)E_x + \gamma D\frac{\partial(n_+ + n_-)}{\partial x}$$

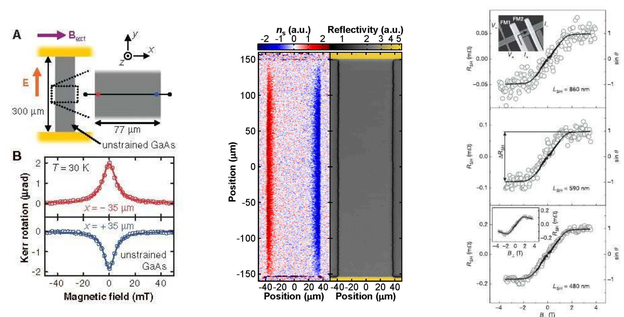
$\mathbf{j}/e = \mu n\mathbf{E} + D\nabla n + \gamma\mu\mathbf{E}\times\mathbf{s} + \gamma D\nabla\times\mathbf{s}$, $S_{ij} = -\mu E_i s_j - D\frac{\partial s_j}{\partial x_i} + \epsilon_{ijk}(\gamma\mu n E_k + \gamma D\nabla_k n)$

anomalous Hall effect (Karplus, Luttinger 1954)
inverse spin-Hall, inhomog. spin density (Averkiev, Dyakonov, Bakun 1983)
Spin-Hall effect charge current induce spin current

Spin-Hall effect

pred.: Dyakonov, Perel 1971, exp:
Kato et al., Science 306 (04) 1910
Sih et. al, Nature Physics 1 (05) 31

anomalous Hall effect
Valenzuela, Tinkham, Nature 442 (06) 176

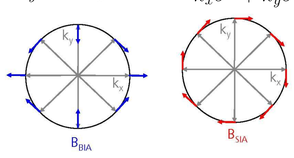


Extrinsic vs intrinsic s.o.

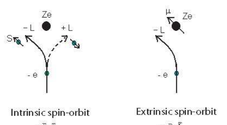
intrinsic: c-band (s) coupled to v-bands (v) GaAs/AlGaAs

bulk-inv. asym. (III-V semicond.) Dresselhaus $-k_y\sigma^y + k_x\sigma^x$

structure inversion asym. (macrosc. confining) Rashba $-k_x\sigma^y + k_y\sigma^x$



General form
$H^s = A(\mathbf{k})\sigma_x - B(\mathbf{k})\sigma_y + C(\mathbf{k})\sigma_z = \mathbf{b}\cdot\sigma$



2D − system	$A(k)$	$B(k)$	$C(k)$
Rashba	$\beta_R k_y$	$\beta_R k_x$	
Dresselhaus[001]	$\beta_D k_x$	$\beta_D k_y$	
Dresselhaus[110]	βk_x	$-\beta k_x$	
Rashba − Dresselhaus	$\beta_R k_y - \beta_D k_x$	$\beta_R k_x - \beta_D k_y$	
cubic Rashba(hole)	$i\frac{\beta_R}{2}(k_-^3 - k_+^3)$	$\frac{\beta_R}{2}(k_-^3 + k_+^3)$	
cubic Dresselhaus	$\beta_D k_x k_y^2$	$\beta_D k_y k_x^2$	
Wurtzite type	$(\alpha + \beta k^2)k_y$	$(\alpha + \beta k^2)k_x$	
single − layer graphene	vk_x	$-vk_y$	
bilayer graphene	$\frac{k_+^2 + k_+^2}{4m_e}$	$\frac{k_+^2 - k_+^2}{4m_e i}$	

3D − system	$A(k)$	$B(k)$	$C(k)$
bulk Dresselhaus	$k_x(k_y^2 - k_z^2)$	$k_y(k_x^2 - k_z^2)$	$k_z(k_x^2 - k_y^2)$
Cooperpairs	Δ	0	$\frac{p^2}{2m} - \epsilon_F$
extrinsic $\beta = \frac{1}{2}\lambda^2 V(k)$	$q_y k_z - q_z k_y$	$q_z k_x - q_x k_z$	$q_x k_y - q_y k_x$
neutrons in nuclei $\beta = iW_0(n_n + \frac{n_p}{2})$	$q_z k_y - q_y k_z$	$q_x k_z - q_z k_x$	$q_y k_x - q_x k_y$

Interactions and meanfields

1. Spin-orbit coupling $\sigma\cdot\mathbf{b}(\mathbf{p})$
magn. impurities, intrinsic+ extrinsic

$$\hat V_{-p,p'} = \begin{cases} V_0(p'-p) \\ \sigma\cdot\mathbf{V}(p'-p) \\ \frac{i\lambda^2}{\hbar}\sigma\cdot(\mathbf{p}\times\mathbf{p}')V(p'-p)\end{cases}$$

2. Leads to impurity meanfields $\Sigma_0^{\rm imp} = nV_0 + \mathbf{s}\cdot\mathbf{V}$; $\mathbf{\Sigma}^{\rm imp} = \mathbf{s}V_0 + n\mathbf{V}$

Extrinsic spin-orbit coupling meanfield more involved
$\Sigma_0^{\rm ext.} = i\frac{\lambda^2}{\hbar^2}V\,[m(\mathbf{S}_j\times\mathbf{q})_j - \mathbf{s}\cdot(\mathbf{p}\times\mathbf{q})]$, $\mathbf{\Sigma}^{\rm ext.} = i\frac{\lambda^2}{\hbar^2}V\,[m(\mathbf{j}\times\mathbf{q}) - n(\mathbf{p}\times\mathbf{q})]$
dens. $n = \sum_p f$, curr. $\mathbf{j} = \sum_p \frac{\mathbf{p}}{m} f$, polar. $\mathbf{s} = \sum_p \mathbf{g}$, curr. $S_{ji} = \sum_p \frac{p_j}{m}[\mathbf{g}]_i$

3. Effective (meanfield) Hamiltonian

$$H = \frac{k^2}{2m} + \Sigma_0(\mathbf{k},\mathbf{q},t) + e\Phi(\mathbf{q},t) + \sigma\cdot\mathbf{\Sigma}(\mathbf{k},\mathbf{q},t)$$

with $\mathbf{\Sigma} = \mathbf{\Sigma}_{MF}(\mathbf{k},\mathbf{q},t) + \mathbf{b}(\mathbf{k},t) + \mu\mathbf{B}$

- Search kinetic theory (non-Abelian) $\int\frac{d\omega}{2\pi}G^< = f(\mathbf{k},\mathbf{q},t) + \sigma\cdot\mathbf{g}(\mathbf{k},\mathbf{q},t)$

Kinetic equation with spin-orbit coupling and electric and magnetic fields

$$(\partial_t + \mathcal{F}\partial_{\mathbf p} + \mathbf{v}\partial_{\mathbf r})f + \mathbf{A}\cdot\mathbf{g} = 0$$
$$(\partial_t + \mathcal{F}\partial_{\mathbf p} + \mathbf{v}\partial_{\mathbf r})\mathbf{g} + \mathbf{A}\,f = 2(\mathbf{\Sigma}\times\mathbf{g})$$

coupling of spinor terms $A_i = \partial_{\mathbf p}\Sigma_i\partial_{\mathbf r} - \partial_{\mathbf r}\Sigma_i\partial_{\mathbf p} + (\partial_{\mathbf p}\Sigma_i\times e\mathbf{B})\partial_{\mathbf p}$
with velocity $\mathbf{v} = \frac{\mathbf k}{m} + \partial_{\mathbf k}\Sigma_0$ and eff. Lorentz force $\mathcal{F} = (e\mathbf{E} - \partial_{\mathbf r}\Sigma_0 + e\mathbf{v}\times\mathbf{B})$

Stationary solution: $\hat\rho(\hat\varepsilon) = \sum_\pm \hat P_\pm f_\pm = \frac{f_+ + f_-}{2} + \sigma\cdot\mathbf{e}\,\frac{f_+ - f_-}{2} = f + \sigma\cdot\mathbf{g}$
with effective splitting $f_\pm = f_0(\epsilon_k \pm |\mathbf{\Sigma}|)$
and selfconsistent meanfield $\epsilon_k(r) = \frac{k^2}{2m} + \Sigma_0(k,r)$
and selfconsistent precession $\mathbf{e}(k,r) = \mathbf{\Sigma}/|\mathbf{\Sigma}|$

Summary on spin transport

- Coupled quantum kinetic equation for spin - $1/2$ - particles including:
  - mean field (scalar+vector) for magnetized impurities, spin-flip, ...
  - arbitrary magnetic and electric fields
  - spin-orbit interaction (nonlinear)
- Anomalous Hall effect, quantum Hall effect, spin-Hall effect and inverse
- Response and collective spin and density modes (staircase)
- Out-of plane polarization follows Landau levels (THz)
- Applications: graphene (pseudospin), optical Hall effects, ...

Particle currents and anomalous Hall effect

$J_\alpha = \sigma^{\rm D}E_\alpha + (\sigma_{\alpha\beta}^{\rm as} + \sigma_{\alpha\beta}^{\rm sym})E_\beta$ with Drude conductivity $\sigma^{\rm D} = \frac{ne^2\tau}{m_e}$ and

$$\left.\begin{matrix}\sigma_{ij}^{\rm as}\\ \sigma_{ij}^{\rm sym}\end{matrix}\right\} = e^2\sum_p\frac{g}{1-\frac{\omega^2}{4|\Sigma|^2}}\begin{cases}\mathbf{e}\cdot(\partial_i\mathbf{e}\times\partial_j\mathbf{e})\\ \frac{i\omega}{2|\Sigma|}\partial_i\mathbf{e}\cdot\partial_j\mathbf{e}\end{cases},\quad \mathbf{e} = \frac{\mathbf\Sigma}{|\Sigma|}, g = \frac12(f_+ - f_-)$$

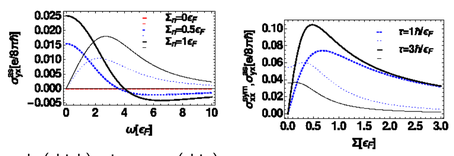
static result agrees with Kubo formula $\sigma_{\alpha\beta} = -\epsilon_{\alpha\beta\gamma}e^2\sum_{np}f_n(\partial_p\times\mathbf{a}_n)_\gamma$

- with Berry-phase connection $\mathbf{a}_n = i\hbar\langle n|\partial_p|n\rangle = \langle n|\mathbf{x}|n\rangle$ for two spin bands $\Sigma_x - i\Sigma_y = \Sigma e^{-i\phi}$ one has $\mathbf{a}_\pm = i\hbar\langle\pm|\partial_p|\pm\rangle = \hbar\frac{\Sigma_\pm\Sigma_z}{2\Sigma}\partial_p\phi$

$T = 0$ linear Rashba, $\mathbf{E}$ in x-direction, $\mathbf{\Sigma}^{\rm MF} + \mu_B\mathbf{B} = \Sigma_n\mathbf{e}_z$

$$\sigma_{yx}^{\rm as} = \frac{e^2}{4\pi\hbar}\Sigma_n\tau_\omega\arctan\left[\frac{2\epsilon_\beta\tau_\omega}{\hbar^2 + 4(2\epsilon_\beta\epsilon_F + \Sigma_n^2)\tau_\omega^2}\right] \to \frac{e^2}{4\pi\hbar}\begin{cases}\frac{\epsilon_\beta\Sigma_n}{2\epsilon_\beta\epsilon_f + \Sigma_n^2} & \omega = 0, \tau\to\infty\\ \frac{\Sigma_n}{\omega}\mathrm{artanh}\left[\frac{2\epsilon_\beta\omega}{\hbar^2\omega^2 - 4(2\epsilon_\beta\epsilon_F + \Sigma_n^2)}\right] & \omega\neq 0, \tau\to\infty\end{cases}$$

with $\epsilon_\beta = m\beta_R^2/\hbar$ and $\tau_\omega = \tau/(1 - i\omega\tau)$



real (thick), imag. (thin) anom. conductivity, $\tau = 0.3\hbar/\epsilon_F$

static anom. (thick) Hall, inv. (thin) Hall conductivity

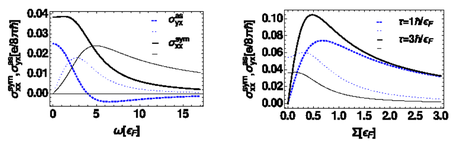
- anomalous Hall vanishes with effective Zeeman, sign change
- static anomalous Hall conductivity has maximum

$m\beta_R^2 = 0.1\epsilon_F$

symmetric part, inverse Hall effect: T=0 $\sigma_{yx}^{\rm sym} = 0$ and

$$\sigma_{xx}^{\rm sym} = \frac{e^2}{16\pi\hbar}\left\{\frac{4\epsilon_\beta\Sigma_n^2\tau_\omega}{2\epsilon_\beta\epsilon_f + \Sigma_n^2} + (1 - 4\Sigma_n^2\tau_\omega^2)\arctan\left[\frac{4\epsilon_\beta\tau_\omega}{\hbar^2 + 4(2\epsilon_\beta\epsilon_F + \Sigma_n^2)\tau_\omega^2}\right]\right\} \approx \frac{e^2}{2\pi\hbar}\frac{\epsilon_\beta\tau}{1 + 4\Sigma_n^2\tau^2} + o(\epsilon_\beta^2)$$

- contribution in direction of electric field caused by collisional correlations
- note $\Sigma_n \to 0$ before expanding: factor 1/2 (symmetry breaking)



real (thick), imag. (thin) dyn. anom. (dashed) and inverse (solid), $\tau = \frac{0.3\hbar}{\epsilon_F}$, $\Sigma_n = 1\epsilon_F$

static anomalous Hall (thick) and inverse Hall conductivity (thin), $m\beta_R^2 = 0.1\epsilon_F$

- static anomalous Hall conductivity vanishes with Zeeman, inverse Hall remains finite
- static conductivities possess maximum
- inverse Hall no sign change, current to electric field direction

Spin currents T=0: $\mathbf{S}_\alpha = -\frac{e\tau}{m_e(1-i\omega\tau)}\mathbf{s}E_\alpha + \sigma_{\alpha\beta}E_\beta$

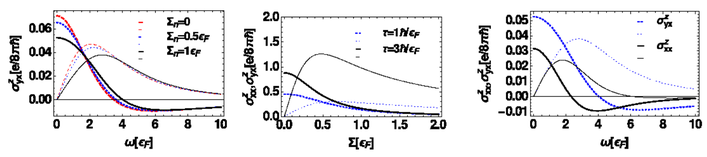
asymmetric (anomalous spin Hall) and symmetric part (inverse spin Hall)

$$\left.\begin{matrix}\sigma_{\alpha\beta}^{\rm as}\\ \sigma_{\alpha\beta}^{\rm sym}\end{matrix}\right\} = \frac{e}{m_e\omega}\sum_p\frac{p_\alpha g}{1 - \frac{\omega^2}{4|\Sigma|^2}}\begin{cases}\frac{i\omega}{2|\Sigma|}\mathbf{e}\times\partial_\beta\mathbf{e}\\ i\partial_\beta\mathbf{e}\end{cases}$$

electric field in x-direction, Rashba (Dresselhaus opposite sign)

$$\sigma_{yx}^z = \frac{e}{8\pi\hbar}\left[1 - \frac{1 + 4\Sigma_n^2\tau_\omega^2}{4\epsilon_\beta\tau_\omega}\arctan\left(\frac{4\hbar\epsilon_\beta\tau_\omega}{\hbar^2 + 4\tau_\omega^2(2\epsilon_\beta\epsilon_F + \Sigma_n^2)}\right)\right],\quad \sigma_{xx}^z = \frac{2}{\hbar}\Sigma_n\tau\sigma_{xy}^z$$

with $\tau_\omega = \tau/(1 - i\omega\tau)$
- universal limit $\sigma_{yx}^z = \frac{e}{8\pi\hbar}\frac{2\epsilon_\beta\epsilon_f}{2\epsilon_\beta\epsilon_f + \Sigma_n^2} + o(1/\tau)$
- necessary for small spin-orbit coupling $\sigma_{yx}^z = \frac{e}{\pi\hbar}\frac{\epsilon_f\tau^2}{(1 - i\omega\tau)^2 + 4\Sigma_n^2\tau^2}\epsilon_\beta + o(\epsilon_\beta^2)$



Real (thick) and imaginary (thin) dynamical spin-Hall coefficient, $\tau = 0.3\hbar/\epsilon_F$

static spin Hall (thick), inverse (thin), Rashba energy of $m\beta_R^2 = 0.1\epsilon_F$

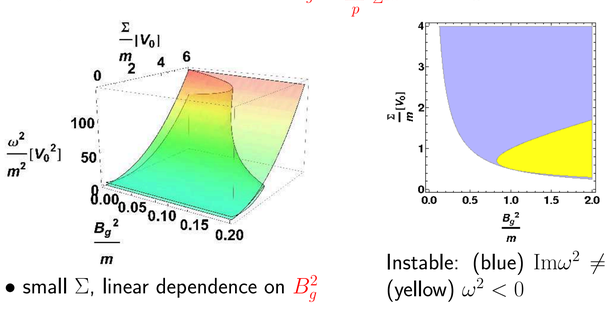
dynamical spin-Hall (solid) and inverse spin-Hall (dashed), $\Sigma_n = 1\epsilon_F$

- spin Hall and inverse spin Hall effect sign change, spin current parallel and antiparallel to electric field direction possible

Linear response

$$(1 - \Pi_0 V_0 - \mathbf{\Pi}\cdot\mathbf{V})\delta n = \Pi_0\Phi^{\rm ext} + (\Pi_0\mathbf{V} + \mathbf{\Pi}V_0)\cdot\delta\mathbf{s}$$
$$[1 - \Pi_0 V_0 - \overleftrightarrow{\Pi}V_0 + \mathbf{\Pi}_3(\mathbf{V}\cdot) + V_0\mathbf{\Pi}_2\times]\delta\mathbf{s} = \mathbf{\Pi}_3\Phi^{\rm ext} + (V_0\mathbf{\Pi}_3 + \Pi_0\mathbf{V} + \mathbf{V}\times\mathbf{\Pi}_2 + \overleftrightarrow{\Pi}\cdot\mathbf{V})\delta n$$

Dipole spin and density waves: neutral impurities
- dipole modes characterized by first-order moments
- density and spin excitation
- analyt. solution: 3 modes with $B_g^2 = \sum_p\frac{b^2}{\Sigma^2}g$ and magnetization $m = s_{q=0}$



- small Σ, linear dependence on B_g^2

Instable: (blue) $\mathrm{Im}\omega^2 \neq 0$, (yellow) $\omega^2 < 0$

K. Morawetz, Europhys. Lett., 104 (2013) 27005
Phys. Rev. **B 92** (2015) 245425
Phys. Rev. **B 92** (2015) 245426
Phys. Rev. **B 94** (2016) 165415

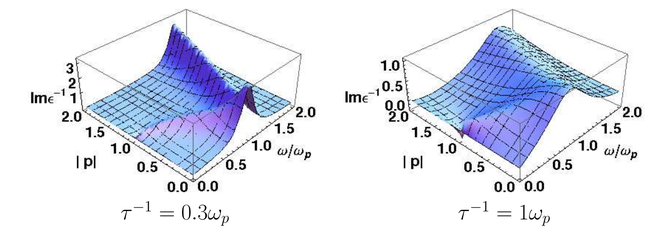
Dipole spin and density waves: charged impurities

- Coulomb potential $V_0 = \frac{e^2}{\epsilon_0 q^2}$ long-wavelength expansion $o(q)$, density eigenmodes: damped plasma oscillation and only transverse spin modes
- dielectric function $\epsilon(\omega,q) = (1 + V_q\chi)^{-1} = 1 - \frac{1}{\frac{1}{1-\epsilon(\omega,0)} - \frac{q^2}{\kappa^{\rm eff}(\omega)}}$

by long-wavelength $\epsilon(\omega,0)$ and dynamical screening length $\kappa^{\rm eff}(\omega)$

$$\epsilon(\omega,0) = \epsilon_\omega + p^2\left(1 - \frac{1}{\epsilon_\omega}\right)\left[1 - \epsilon_\omega - \frac{B_f^2}{\epsilon_\omega}\left((1-\epsilon_\omega)^2 - \frac{\omega_p^2}{\omega^2(1+p^2)}\right)\right]$$

Drude $\epsilon_\omega = 1 - \frac{\omega_p^2}{\omega(\omega + \frac{i}{\tau})}$, eff. pol. $p = \frac{s}{n} = \frac{n_\uparrow - n_\downarrow}{n} - \frac{B_g^2}{2n}$, $B_g^2 = \frac{2p}{1+p^2}B_f^2$

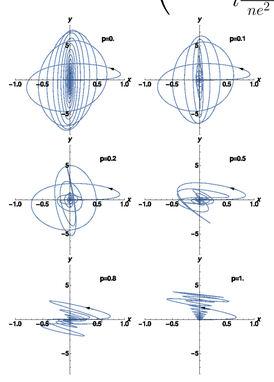


$\tau^{-1} = 0.3\omega_p$ $\tau^{-1} = 1\omega_p$

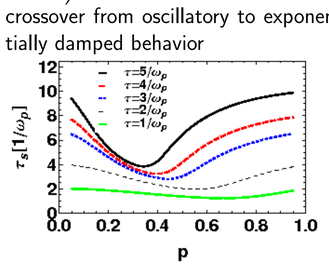
- Instability for $\epsilon^{-1} < 0$ spin domain separation (segregation)

Spin response to external electric field

$$\frac{\delta\mathbf{s}_q}{E} = i\frac{e}{q}\chi_s = \frac{en}{\omega_p}\begin{pmatrix} s_1(\omega)\frac{b_1(q)}{q} + B_c s_2(\omega)\frac{b_2(q)}{q}\\ s_1(\omega)\frac{b_2(q)}{q} - B_c s_2(\omega)\frac{b_1(q)}{q}\\ i\frac{q\epsilon_0\omega_p}{ne^2}s_3(\omega)\end{pmatrix},\quad B_c = \frac{\omega_c\epsilon_f}{nD\hbar\omega_p^2} = \epsilon_0\frac{B}{nDe\hbar}\frac{\epsilon_f}{n}$$



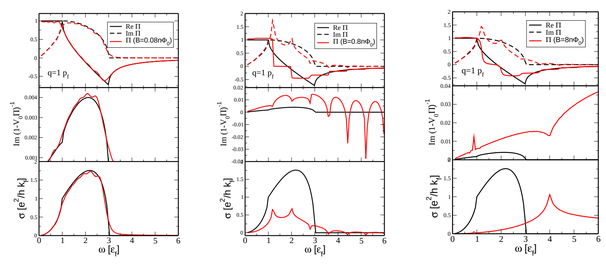
crossover from oscillatory to exponentially damped behavior



spin dephasing time for s_1
$\mathbf{E}$ in x-direction, $\tau^{-1} = 0.1\omega_p$, $B_c = 1$

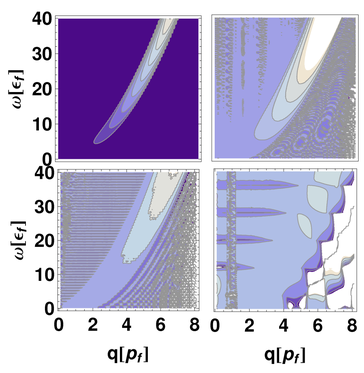
Linear response special cases: magnetic field, no spin

Magnetic field-dependent response $\delta n = \kappa\Phi^{\rm ext}$
corresponding to GW (RPA, rainbow, ...), $n = 7\times10^{10}{\rm cm}^{-2}$
$\kappa(q\omega) = \frac{\Pi_0(q,\omega)}{1 - V_0(q)\Pi_0(q,\omega)}$, $\sigma = -i\omega\epsilon_0\epsilon$, $\epsilon = 1 - V_0\Pi_0$



real (solid red) and imaginary part (dashed red) of response function (above) together with zero magnetic field ones (black lines), excitation (middle) and dynamical conductivity (below) for different magnetic fields (flux $\Phi_0 = h/2e$)

Collective density excitation
$\mathrm{Im}\,(1 - V_0\Pi_0)^{-1}$ measure for position and width of mode $\omega = \omega_0 + I\Gamma$
excitation spectrum for $B = 0, 0.08\Phi_0$n (above) and $B = 0.8, 8\Phi_0$n (below)



Linear response special cases: no magn. impurities

no spin-flip mechanism $\mathbf{V} = 0$, spin excitation influences density response only for asymmetric momentum distributions 2D with $\mathbf{s} = (s_x^0, s_y^0, 0)$, $\mathbf{g}(p) = \mathbf{s}f_0(p)$ follows $\mathbf{\Pi}_3\cdot\mathbf{\Pi} = \mathbf{\Pi}^2 = \Pi_0^2$

$$\delta\mathbf{s} = \frac{\mathbf{\Pi}_3}{1 - 2V_o\Pi_o}U^{\rm ext},\qquad \delta n = \frac{\Pi_0}{1 - 2V_o\Pi_o}U^{\rm ext}$$

and vector polarization for Dresselhaus (Rashba) linear spin-orbit coupling

$$\mathbf{\Pi}_3 = \mathbf{s}\Pi_0 + \mathbf{s}\times\mu\mathbf{B}\Pi_0' - \left(0, 0, \beta s_y^0 - \alpha s_x^0\right)\Pi_{0cos}'$$

out of plane polarization induced by spin precession
for Dresselhaus (Rashba) linear spin-orbit coupling