8.322: Quantum Theory II

Problem Set #12 Solutions
May 18, 2007

1. **Scattering on a strip and the Landauer conductivity**

   (a) The 2D Schrödinger equation

$$-\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\psi(x,y)+V(x,y)\ \psi(x,y)=k^2\psi(x,y)$$

Now we plug in the expansion

$$\psi(x,y)=\sum_{n=1}^{\infty}\sqrt{2}\sin(n\pi y)\psi_n(k,x)$$

($k^2=2mE$ is the electron energy) to obtain

$$-\sum_{n=1}^{\infty}\sqrt{2}\sin(n\pi y)\psi_n''(k,x)+\sum_{n=1}^{\infty}(n\pi)^2\sqrt{2}\sin(n\pi y)\psi_n(k,x)+$$

$$+V(x,y)\sum_{n=1}^{\infty}\sqrt{2}\sin(n\pi y)\psi_n(k,x)=k^2\sum_{n=1}^{\infty}\sqrt{2}\sin(n\pi y)\psi_n(k,x)$$

Defining

$$V_{nm}(x)=\int 2\sin(n\pi y)V(x,y)\sin(m\pi y)dy$$

we can rewrite the Schrödinger equation as

$$\sum_{n=1}^{\infty}\sqrt{2}\sin(n\pi y)\left(-\psi_n''(k,x)+(n\pi)^2\psi_n(k,x)+\sum_{m=1}^{\infty}V_{nm}(x)\psi_m(k,x)-k^2\psi_n(k,x)\right)=0$$

By orthonormality of the sine function, the above holds iff

$$-\psi_n''(k,x)+\sum_{m=1}^{\infty}V_{nm}(x)\psi_m(k,x)=(k^2-n^2\pi^2)\psi_n(k,x)$$

Hence, the 2D Schrödinger equation is equivalent to an infinite set of coupled 1D equations.

(b) $m_{\rm max}$ is the highest open channel, i.e. the largest m for which

$$\Phi_m(\pm k, x) = \frac{1}{\sqrt{k_m}} \begin{pmatrix} 0 \\ \vdots \\ e^{\pm i k_m x} \\ \vdots \end{pmatrix}$$

propagates to infinity. This happens when

$$k_m = \sqrt{k^2 - m^2\pi^2}$$

is real, that is if $k^2 > m^2\pi^2$.

(c) Consider the case when the incoming wave is $\Phi_n(k, x)$. The wave comes from the left and the total incoming flux at $x \ll -d$ is

$$I_{\rm in} = \int 2 \;{\rm Im}\left(\psi(x,y)^* \vec{\nabla}\psi(x,y)\right) \cdot \hat{n}\; dS = \int_0^1 2\;{\rm Im}\left(\psi(x,y)^* \frac{\partial}{\partial x}\psi(x,y)\right) dy$$

$$= 2\int_0^1 2\sin^2(n\pi y) dy = 2$$

The total outgoing flux to the right is

$$I_{\text{out, right}} = 2\int_0^1 {\rm Im}\left(\psi^* \frac{\partial \psi}{\partial x}\right) dy$$

where

$$\psi(x,y) \approx \sum_{l=1}^{\infty} \sqrt{2}\sin(l\pi y)\langle x| \sum_{m}^{m_{max}} T_{mn}(k)\Phi_m(k,x)\rangle = \sum_{m=1}^{m_{max}} \sqrt{2}\sin(m\pi y) T_{mn}(k) \frac{1}{\sqrt{k_m}} e^{ik_m x}$$

Hence,

$$I_{\text{out, right}} = 2\sum_{m=1}^{m_{max}}\sum_{m'=1}^{m_{max}} \left(2\sin(m\pi y)\sin(m'\pi y) dy\right) {\rm Im}\left(T_{m'n}(k)^* T_{mn}(k) i\sqrt{\frac{k_m}{k_{m'}}} e^{i(k_m - k_{m'})x}\right)$$

$$= 2\sum_{m=1}^{m_{max}} {\rm Re}\left(T_{mn}(k)^* T_{mn}(k)\right) = 2\sum_{m=1}^{m_{max}} |T_{mn}(k)|^2$$

The total outgoing flux to the left is

$$I_{\text{out, left}} = -2\int_0^1 {\rm Im}\left(\psi^* \frac{\partial \psi}{\partial x}\right) dy$$

where

$$\psi(x,y) \approx -\sum_{l=1}^{\infty} \sqrt{2}\sin(l\pi y)\langle x| \sum_{m}^{m_{max}} R_{mn}(k)\Phi_m(-k,x)\rangle = -\sum_{m=1}^{m_{max}} \sqrt{2}\sin(m\pi y) R_{mn}(k) \frac{1}{\sqrt{k_m}} e^{-ik_m x}$$

Thus,

$$I_{\text{out, left}} = 2\sum_{m=1}^{m_{max}} |R_{mn}(k)|^2$$

By conservation of flux,

$$I_{\text{in}} = I_{\text{out, left}} + I_{\text{out, right}}$$

Therefore,

$$1 = \sum_m (|T_{mn}|^2 + |R_{mn}|^2)$$

(d) The Lippmann–Schwinger equation is

$$\psi_{nm}^{(+)}(x) = \frac{1}{\sqrt{k_n}}\delta_{mn}e^{ik_nx} + \sum_{m'}\int G_m(k;x,x')V_{mm'}(x')\psi_{m'n}^{(+)}(k,x')dx'$$

with

$$\delta_{mm'}G_m(k;x,x') = \langle m,x|\frac{1}{k^2 - H_0 + i\epsilon}|m',x'\rangle$$

(e) We have

$$\frac{d^2}{dx^2}G_n(k;x,x') + (k^2 - n^2\pi^2)G_n(k;x,x') = \delta(x-x')$$

The solution is

$$G_n(k;x,x') = \frac{1}{2k_n}\sin(k_n|x-x'|) + A\sin(k_n|x-x'|) + B\cos(k_n|x-x'|)$$

From the boundary conditions ($G_n \to e^{ik_n(x-x')}$), we have $A = 0$ and $B = 1/2ik_n$ and

$$G_n(k;x,x') = \frac{1}{2ik_n}e^{ik_n|x-x'|}$$

(f) From the Lippmann–Schwinger equation,

$$\psi_{mn}^{(+)}(x) = \frac{1}{\sqrt{k_n}}\delta_{mn}e^{ik_nx} + \sum_{m'=1}^{\infty}\frac{1}{2i}\int\frac{1}{k_m}e^{ik_m|x-x'|}V_{mm'}(x')\psi_{m'n}^{(+)}(x')dx'$$

When $x \to \infty$,

$$\psi_{mn}^{(+)}(x) \longrightarrow \frac{1}{\sqrt{k_n}}\delta_{mn}e^{ik_nx} + \frac{e^{ik_mx}}{\sqrt{k_m}}\sum_{m'=1}^{m_{max}}\frac{1}{2i}\int_{-d}^{d}\frac{1}{\sqrt{k_m}}e^{-ik_mx'}V_{mm'}(x')\psi_{m'n}^{(+)}(x')dx'$$

Comparing with the definition of T_{mn}, we have

$$T_{mn}(k) = \delta_{mn} + \sum_{m'=1}^{m_{max}}\frac{1}{2i}\int_{-d}^{d}\frac{1}{\sqrt{k_m}}e^{-ik_mx'}V_{mm'}(x')\psi_{m'n}^{(+)}(x')dx'$$

When $x \to -\infty$,

$$\psi_{mn}^{(+)}(x) \longrightarrow \frac{1}{\sqrt{k_n}}\delta_{mn}e^{ik_nx} + \frac{e^{-ik_mx}}{\sqrt{k_m}}\sum_{m'=1}^{m_{max}}\frac{1}{2i}\int_{-d}^{d}\frac{1}{\sqrt{k_m}}e^{ik_mx'}V_{mm'}(x')\psi_{m'n}^{(+)}(x')dx'$$

Comparing with the definition of R_{mn}, we have

$$R_{mn}(k) = -\sum_{m'=1}^{m_{max}}\frac{1}{2i}\int_{-d}^{d}\frac{1}{\sqrt{k_m}}e^{ik_mx'}V_{mm'}(x')\psi_{m'n}^{(+)}(x')dx'$$

(g) In the first Born approximation,

$$R_{mn}(k) = -\sum_{m'=1}^{m_{max}}\frac{1}{2i}\int_{-d}^{d}\frac{e^{i(k_m+k_n)x'}}{\sqrt{k_mk_n}}V_{mn}(x')dx'$$

$$T_{mn}(k) = \delta_{mn} + \sum_{m'=1}^{m_{max}}\frac{1}{2i}\int_{-d}^{d}\frac{e^{i(k_n-k_m)x'}}{\sqrt{k_mk_n}}V_{mn}(x')dx'$$

(h) If $V_{mn}(x) = 0$, then $T_{mn}(k) = \delta_{mn}$. Hence,

$$\mathrm{Tr}\left[T^{\dagger}(k_F)T(k_F)\right] = \dim T(k_F) = m_{\max}$$

and

$$\sigma(k_F) = \frac{2e^2}{h}m_{\max}(k_F)$$

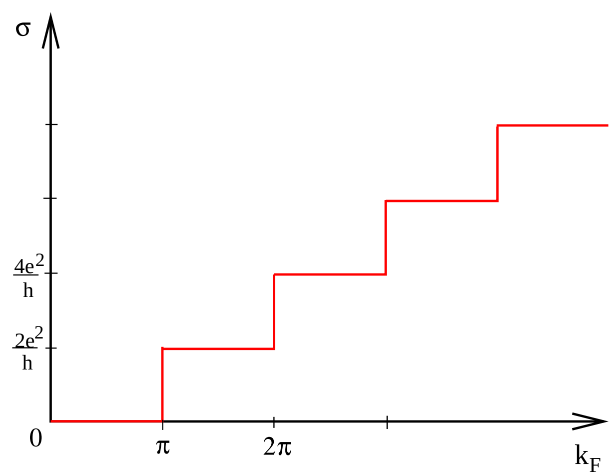

Figure 1: σ as a function of k_F.

2. **Analyzing a scattering amplitude**

(a) In general,

$$f(k,\theta) = \sum_{l=0}^{\infty}(2l+1)f_l(k)P_l(\cos\theta)$$

From the form of the given scattering amplitude

$$f(k,\theta) = \frac{1}{k}\left(\frac{g(k)}{k_0 - k - i\Gamma} + Ae^{2i\beta h(k)}\sin(2\beta h(k))\cos\theta\right)$$

clearly, $l = 0, 1$ are active.

(b) The partial wave is related to the corresponding S–matrix component by

$$S_l(k) = 1 + 2ikf_l(k)$$

From $f(k,\theta)$ we have

$$f_0(k) = \frac{1}{k}\frac{g(k)}{k_0 - k - i\Gamma}$$

and the unitarity constraint is

$$1 = S_0^*(k)S_0(k) = \left(1 + \frac{2ig(k)}{k_0 - k - i\Gamma}\right)^*\left(1 + \frac{2ig(k)}{k_0 - k - i\Gamma}\right) = 1 + \frac{4g(k)^2 - 4\Gamma g(k)}{(k-k_0)^2 + \Gamma^2}$$

from which $g(k) = 0$ or Γ. We keep the nontrivial solution

$$g(k) = \Gamma$$

Next, we can read off

$$f_1(k) = \frac{A}{3k}e^{2i\beta h(k)}\sin(2\beta h(k))$$

On the other hand,

$$f_1(k) = \frac{1}{k}e^{i\delta_1(k)}\sin(\delta_1(k))$$

from which we get

$$A = 3$$

Also,

$$2\beta h(k) = \delta_1(k)$$

At small k,

$$\delta_l \approx \tan\delta_l \sim (kR)^{2l+1}$$

and thus

$$2\beta h(k) \sim k^3$$

Hence,

$$h(k) \sim k^3$$

(c) For $l = 0$,

$$\frac{e^{2i\delta_0} - 1}{2ik} = \frac{1}{k}\frac{g(k)}{k_0 - k - i\Gamma}$$

Hence,

$$e^{2i\delta_0} = \frac{k_0 - k + i\Gamma}{k_0 - k - i\Gamma}$$

and

$$\delta_0 = \frac{1}{2i} \ln\left(\frac{k_0 - k + i\Gamma}{k_0 - k - i\Gamma}\right)$$

For $l = 1$, we have seen that

$$\delta_1(k) = 2\beta h(k)$$

(d) The differential cross section is

$$\frac{d\sigma}{d\Omega} = |f|^2 = \frac{1}{k^2}\left|\frac{\Gamma}{k_0 - k - i\Gamma} + 3e^{2i\beta h(k)} \sin(2\beta h(k)) \cos\theta\right|^2$$

(e) Generically,

$$\sigma_l = 4\pi(2l+1) \cdot |f_l(k)|^2$$

Here

$$\sigma_0 = 4\pi|f_0|^2 = \frac{4\pi}{k^2}\frac{\Gamma^2}{(k_0-k)^2+\Gamma^2}$$

$$\sigma_1 = 4\pi \cdot 3 \cdot |f_0|^2 = \frac{12\pi}{k^2}\sin^2(2\beta h(k))$$

(f) The total cross section is

$$\sigma_{\text{total}} = \sum_l \sigma_l = \sigma_0 + \sigma_1 = \frac{4\pi}{k^2}\frac{\Gamma^2}{(k_0-k)^2+\Gamma^2} + \frac{12\pi}{k^2}\sin^2(2\beta h(k))$$

As $k \approx k_0$, we have

$$\sigma_{\text{total}} = \frac{4\pi}{k_0^2} + \frac{12\pi}{k_0^2}\sin^2(2\beta h(k_0)) - \frac{4\pi}{k_0^2}\frac{(k_0-k)^2}{\Gamma^2}$$

(The last term may be zero.)

(g) For general k, we have again

$$\sigma_{\text{total}}(k) = \frac{4\pi}{k^2}\frac{\Gamma^2}{(k_0-k)^2+\Gamma^2} + \frac{12\pi}{k^2}\sin^2(2\beta h(k))$$

The imaginary part of the forward scattering amplitude is

$$\text{Im } f(k,0) = \frac{1}{k}\left[\frac{\Gamma^2}{(k_0-k)^2+\Gamma^2} + 3\sin^2(2\beta h(k))\right]$$

We see that

$$\sigma_{\text{total}} = \frac{4\pi}{k}\text{Im } f(k,0)$$

and the optical theorem holds.

3. **Scattering of thermal neutrons - Wigner's $\mathcal{R}$ Matrix Method**

(a)

$$\lambda_{\text{de Broglie}} = \frac{h}{p} = \frac{h}{\sqrt{2mE}} \approx 0.175 \text{ nm}$$

(b) The angular momentum barrier prevents neutrons probing the core potential when $l \neq 0$.

(c) Let $u(r)$ and $w(r)$ be two wavefunctions satisfying the boundary conditions

$$\left.\frac{u}{u'}\right|_{r=0} = \mathcal{R} \qquad \left.\frac{w}{w'}\right|_{r=0} = \mathcal{R}$$

For H to be Hermitian, we need

$$\int_0^\infty u(r)^*[Hw(r)]\ dr = \int_0^\infty [Hu(r)]^* w(r)\ dr$$

which is

$$\int_0^\infty u^*(r)(-w''(r))\ dr = \int_0^\infty (-u''(r))^* w(r)\ dr$$

Integrating by parts gives

$$\int_0^\infty u^*(r)(-w''(r))\ dr = [-u^*(r)w'(r) + u'(r)^* w(r)]_0^\infty + \int_0^\infty (-u''(r))^* w(r)\ dr$$

Thus we need

$$[-u^*(r)w'(r) + u'(r)^* w(r)]_0^\infty = 0$$

This is satisfied iff

$$\left(\frac{u(0)}{u'(0)}\right)^* \left(\frac{w'(0)}{w(0)}\right) = 1$$

that is

$$\mathcal{R}^* \cdot \frac{1}{\mathcal{R}} = 1$$

Hence, H is Hermitian provided that $\mathcal{R}$ is real.

(d) With $V(r) = 0$ for $r > 0$, the Schrödinger equation becomes

$$-u''(r) = k^2 u(r)$$

with solution

$$u(r) = A \sin(kr + \delta_0(k))$$

Then,

$$u'(r) = Ak \cos(kr + \delta_0(k))$$

and

$$\mathcal{R} = \frac{u(0)}{u'(0)} = \frac{\tan(\delta_0(k))}{k}$$

Thus,

$$\delta_0(k) = \arctan(k\mathcal{R})$$

(e) The S–matrix

$$S_0(k) = e^{2i\delta_0(k)} = e^{2i\arctan(k\mathcal{R})} = \frac{1 - ik\mathcal{R}}{1 + ik\mathcal{R}}$$

For $k = i\kappa$,

$$S_0(i\kappa) = e^{-2\operatorname{artanh}(\kappa\mathcal{R})}$$

Note that $\operatorname{artanh}(x) \to -\infty$ as $x \to -1$. Hence, S_0 has a pole at $k = 1/i\mathcal{R}$, i.e. when $\kappa = -1/\mathcal{R}$.

Recall that

$$u(r) = A\left(e^{-ikr} - e^{2i\delta_0(k)}e^{ikr}\right) = A\left(e^{-ikr} - e^{2i\arctan(k\mathcal{R})}e^{ikr}\right)$$

Thus we have

$$\phi(r) = \lim_{k\to i\kappa}(k - i\kappa)u(r) \sim e^{i(i\kappa)r} = e^{-\kappa r}$$

Therefore if $\kappa > 0$, then $\phi(r)$ is normalizable. The wavefunction is concentrated around $r = 0$. It corresponds to a bound state of the neutron. The energy of the state is

$$E = \frac{k^2}{2m} = -\frac{\kappa^2}{2m} = -\frac{1}{2m\mathcal{R}^2}$$

In order for Wigner's $\mathcal{R}$–theory to be reliable, the wavefunction must extend to a large length scale w.r.t. R_N. That is $|\mathcal{R}| \gg R_N$. In terms of the energy,

$$|E| = \frac{1}{2m\mathcal{R}^2} \ll \frac{1}{2mR_N^2}$$

(f) The total cross section is

$$\sigma(k, \mathcal{R}) \approx 4\pi|f_0(k, \mathcal{R})|^2 = \frac{4\pi}{k^2}\sin^2(\delta_0(k)) = \frac{4\pi}{k^2}\cdot\frac{k^2\mathcal{R}^2}{1 + k^2\mathcal{R}^2}$$

When the bound state approaches the threshold, we have

$$\frac{1}{2m\mathcal{R}^2} \longrightarrow 0$$

and thus

$$\mathcal{R} \longrightarrow -\infty$$

Hence, around the threshold

$$\sigma(k) \approx \frac{4\pi}{k^2}$$

so the cross section diverges as the bound state approaches threshold.

4. **Spin dependent scattering**

(a) From the last problem set we know

$$f_{ss'}(\vec{k},\vec{k}') = -\frac{2m}{4\pi}\langle\vec{k}',s'|V|\vec{k},s\rangle = -\frac{2m}{4\pi}\langle\vec{k}',s'|V(r)+\frac{1}{2m^2c^2r}\frac{dV}{dr}\vec{L}\cdot\vec{S}|\vec{k},s\rangle$$

$$= -\frac{2m}{4\pi}\left(\langle\vec{k}'|V(r)|\vec{k}\rangle\delta_{ss'} + \frac{1}{2m^2c^2}\langle\vec{k}'|\frac{1}{r}\frac{dV}{dr}\vec{L}|\vec{k}\rangle\cdot\langle s'|\vec{S}|s\rangle\right)$$

$$= -\frac{2m}{4\pi}\left(\delta_{ss'}\int d^3\vec{x}\ e^{i(\vec{k}-\vec{k}')\cdot\vec{x}}V(\vec{x}) + \frac{1}{2m^2c^2}\vec{S}\cdot\int d^3\vec{x}\ e^{i(\vec{k}-\vec{k}')\cdot\vec{x}}\frac{1}{r}\frac{dV}{dr}\vec{x}\times\vec{k}\right)$$

$$= -\frac{2m}{4\pi}\left(\underbrace{\delta_{ss'}\frac{4\pi}{q}\int_0^\infty rV(r)\sin\ qr\ dr}_{\tilde{V}(q^2)} + \frac{2\pi}{2m^2c^2}\vec{S}\cdot\int r^2dr\ \frac{dV}{dr}2i\left(\frac{\cos\ qr}{qr}-\frac{\sin\ qr}{(qr)^2}\right)\hat{q}\times\vec{k}\right)$$

$$= -\frac{2m}{4\pi}\left(\tilde{V}(q^2) + \underbrace{\frac{4\pi i}{2m^2c^2q}\int r^2dr\ \frac{dV}{dr}\left(\frac{\sin\ qr}{(qr)^2}-\frac{\cos\ qr}{qr}\right)}_{\tilde{V}_{SO}(q^2)}(\vec{k}\times\vec{k}')\cdot\vec{S}\right)$$

$$= -\frac{2m}{4\pi}\left(\tilde{V}(q^2)+\tilde{V}_{SO}(q^2)(\vec{k}\times\vec{k}')\cdot\vec{S}\right)$$

where

$$\tilde{V}(q^2) = \delta_{ss'}\frac{4\pi}{q}\int_0^\infty rV(r)\sin\ qr\ dr$$

$$\tilde{V}_{SO}(q^2) = \frac{4\pi i}{2m^2c^2q}\int r^2dr\ \frac{dV}{dr}\left(\frac{\sin\ qr}{(qr)^2}-\frac{\cos\ qr}{qr}\right)$$

(b) The spin averaged differential cross section is

$$\langle\frac{d\sigma}{d\Omega}\rangle = \langle|f_{ss'}(\vec{k},\vec{k}')|^2\rangle_{ss'} = \left(\frac{2m}{4\pi}\right)^2\langle|\tilde{V}(q^2)+\tilde{V}_{SO}(q^2)(\vec{k}\times\vec{k}')\cdot\vec{S}|^2\rangle_{ss'}$$

Since $\tilde{V}$ is real and $\tilde{V}_{SO}$ is imaginary,

$$\langle\frac{d\sigma}{d\Omega}\rangle = \left(\frac{2m}{4\pi}\right)^2\left(\tilde{V}^2(q^2)+|\tilde{V}_{SO}(q^2)|^2\langle[(\vec{k}\times\vec{k}')\cdot\vec{S}]^2\rangle_{ss'}\right)$$

Finally, we have

$$\langle[(\vec{k}\times\vec{k}')\cdot\vec{S}]^2\rangle_{ss'} = \frac{1}{2}\sum_{ss'}\langle s'|\left((\vec{k}\times\vec{k}')\cdot\vec{S}\right)\left((\vec{k}\times\vec{k}')\cdot\vec{S}\right)|s\rangle$$

$$= \frac{1}{2}\sum_{ss's_i}\langle s'|(\vec{k}\times\vec{k}')\cdot\vec{S}|s_i\rangle\ \langle s_i|(\vec{k}\times\vec{k}')\cdot\vec{S}|s\rangle = \frac{1}{4}(\vec{k}\times\vec{k}')^2$$

So

$$\langle\frac{d\sigma}{d\Omega}\rangle = \left(\frac{2m}{4\pi}\right)^2 \left(\tilde{V}^2(q^2) + |\tilde{V}_{SO}(q^2)|^2 \frac{(\vec{k}\times\vec{k}')^2}{4}\right) = \frac{m^2}{4\pi^2}\left(\tilde{V}^2(q^2) + |\tilde{V}_{SO}(q^2)|^2 \frac{k^4 \sin^2\theta_{\vec{k},\vec{k}'}}{4}\right)$$

(c) An unpolarized particle is described by the density matrix

$$\rho_0 = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$$

If we regard the scattering amplitude as a matrix function of $\vec{k}$ and $\vec{k}'$,

$$f(\vec{k},\vec{k}') = -\frac{2m}{4\pi}\left(\tilde{V}(q^2)\mathbb{1} + \frac{1}{2}\tilde{V}_{SO}(q^2)(\vec{k}\times\vec{k}')\cdot\vec{\sigma}\right)$$

If we look at scattering into a specified $\vec{k}'$, then each incident spin state $|s\rangle$ is mapped into a final spin state $f|s\rangle$. The density matrix thus goes to

$$\rho_0 \longrightarrow \rho_s = \frac{f\rho_0 f^\dagger}{\mathrm{Tr}(f\rho_0 f^\dagger)}$$

Defining the polarization as $\vec{P} = \mathrm{Tr}(\vec{\sigma}\rho_s)$, we have

$$\vec{P} = \mathrm{Tr}\left(\vec{\sigma}\frac{f\rho_0 f^\dagger}{\mathrm{Tr}(f\rho_0 f^\dagger)}\right)$$

Plugging in f, we obtain

$$\vec{P} = \frac{\mathrm{Re}\left[\tilde{V}(q^2)\tilde{V}^*_{SO}(q^2)\right](\vec{k}\times\vec{k}')}{|\tilde{V}(q^2)|^2 + \frac{1}{4}|\tilde{V}_{SO}|^2(\vec{k}\times\vec{k}')}$$

so the polarization is normal to the scattering plane and vanishes for forward scattering.