Nontrivial contributions to the magnetoconductivity due to anomalous $g$-factor in the Luttinger Hamiltonian

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Abstract. The effective $g$-factor and the selection rules for the matrix elements of the velocity operator are investigated for the Luttinger Hamiltonian under a magnetic field. It is shown that the $g$-factor has a strong $k_z$-dependence, where $k_z$ is the wave vector along the magnetic field. This anomalous $k_z$-dependence is due to the interband effect of the magnetic field between the light and heavy hole bands. It is found that a nontrivial contribution to the longitudinal magnetoconductivity arises also due to the interband effects by analyzing the selection rules. This nontrivial interband contribution can be a source of the longitudinal spin current.

1. Introduction
The Luttinger Hamiltonian was introduced first as an effective Hamiltonian for semiconductors such as Si or Ge [1]. In these semiconductors, three bands are degenerate at $k = 0$ when there is no spin-orbit interaction (SOI) and effects of electron spin are neglected. If the SOI is present, these three degenerate bands (sixfold due to spins) breaks up into one fourfold and one twofold bands. The fourfold band lies higher than the twofold one and it is more important in practice. The Luttinger Hamiltonian is the effective Hamiltonian derived for this fourfold band on the basis of $k \cdot p$ theory. It is written in terms of $4 \times 4$ matrix. The Luttinger Hamiltonian is valid also for semiconductors such as GaAs and InSb at temperatures higher than the energy scale of the band splitting originated from the lack of the inversion symmetry [2]. Thus the Luttinger Hamiltonian is the most fundamental effective Hamiltonian in semiconductor physics. Moreover, the Luttinger Hamiltonian has attracted revived interests since the proposal of intrinsic spin Hall effect in the Luttinger Hamiltonian [3, 4].

In addition, the relationship to the Dirac Hamiltonian, which is also written in terms of $4 \times 4$ matrix, is an interesting subject. In some materials with a strong SOI, such as Bi and PbTe, the effective Hamiltonian is essentially equivalent to the Dirac Hamiltonian except for a spatial anisotropy [5, 6]. It was found that the Dirac Hamiltonian also exhibits the intrinsic spin Hall effect [7, 8]. Therefore, the Luttinger and Dirac Hamiltonian should share common features since both of them are written in terms of $4 \times 4$ matrix and the interband matrix elements due to the SOI plays crucial roles. But it has not been clearly understood yet.

The purpose of the present work is to revisit the Luttinger Hamiltonian and study the quantum transport phenomena paying special attention to the anomalous property of $g$-factor.
in the Luttinger Hamiltonian. It is well known that the effective $g$-factor can be greatly different from the value for bare electrons ($g = 2$) when there is a SOI [1, 9–11]. Actually, the effective $g$-factor of Bi can exceed 1000 due to the strong SOI [6, 12]. Furthermore, the effective $g$-factor can be $k$-dependent. It was approximately shown [11] that the effective $g$-factor of the Luttinger Hamiltonian exhibit a linear-$k_z$ dependence for large quantum numbers of Landau levels as $g^* \propto |k_z|$, where $k_z$ is the wave vector along the magnetic field.

Here we propose that an interesting spin transport will emerge with such a $k$-dependent effective $g$-factor. For example, suppose the effective Hamiltonian is given as

$$
\mathcal{H} = \frac{\hbar^2 k^2}{2m} + \frac{g^*(k_z)}{2} \mu_B \sigma \cdot B,
$$

where $\mu_B = e\hbar/2mc$ is the Bohr magneton, $\sigma$ is the Pauli spin matrix, and $B$ is an external magnetic field. The second term of Eq. (1) is the effective Zeeman term originates from the orbital motion of electrons (not the bare Zeeman term). In general cases, $g^*$ is independent from $k_z$, so that the current $j_i = ev_i = e\partial \mathcal{H}/\hbar\partial k_i$ is independent from $g^*$ and the spin. ($e$ is the elementary charge and $v_i$ is the velocity along the $i$-direction.) By contrast, in the case that $g^*$ depends on $k_z$, the current is different between opposite spins as

$$
j_{z\uparrow,\downarrow} = ev_z(k_z) \pm \frac{e\mu_B B_z \partial g^*(k_z)}{2\hbar} \frac{\partial g^*(k_z)}{\partial k_z}.
$$

This suggests that the spin current, $j_{z\uparrow} = j_{z\uparrow} - j_{z\downarrow}$, can flow along the magnetic field when the $g^*$ depends on $k_z$. Of course, the above argument based on the quasi-classical picture is too naive to discuss the spin transport phenomena, which is the essentially quantum phenomena. In order to examine this idea, we need to study the magnetoconductivity based on the quantum transport theory.

2. Model

The Luttinger Hamiltonian under a magnetic filed is given by

$$
\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 + \mathcal{H}_2,
$$

$$
\mathcal{H}_0 = \frac{1}{2m} \left( \begin{array}{cc} \mathcal{H}_0' & 0 \\ 0 & \mathcal{H}_0'' \end{array} \right),
$$

$$
\mathcal{H}_0' = \left( \begin{array}{cc} (\gamma_1 + \gamma)(\pi_x^2 + \pi_y^2) + 3\hbar^2 s\kappa & -3\sqrt{3}\gamma(\pi_x - i\pi_y) \\ -3\sqrt{3}\gamma(\pi_x + i\pi_y) & (\gamma_1 - \gamma)(\pi_x^2 + \pi_y^2) - \hbar^2 s\kappa \end{array} \right),
$$

$$
\mathcal{H}_0'' = \left( \begin{array}{cc} (\gamma_1 - \gamma)(\pi_x^2 + \pi_y^2) + \hbar^2 s\kappa & -3\sqrt{3}\gamma(\pi_x - i\pi_y) \\ -3\sqrt{3}\gamma(\pi_x + i\pi_y) & (\gamma_1 + \gamma)(\pi_x^2 + \pi_y^2) - \hbar^2 s\kappa \end{array} \right),
$$

$$
\mathcal{H}_1 = \frac{1}{2m} \left( \begin{array}{cccc} (\gamma_1 - 2\gamma)\pi_x^2 & 0 & 0 & 0 \\ 0 & (\gamma_1 + 2\gamma)\pi_x^2 & 0 & 0 \\ 0 & 0 & (\gamma_1 + 2\gamma)\pi_z^2 & 0 \\ 0 & 0 & 0 & (\gamma_1 - 2\gamma)\pi_z^2 \end{array} \right),
$$

$$
\mathcal{H}_2 = \frac{1}{2m} \left( \begin{array}{cccc} 0 & 0 & -2\gamma\sqrt{3}(\pi_x - i\pi_y)\pi_z & 0 \\ 0 & 0 & 0 & 2\gamma\sqrt{3}(\pi_x - i\pi_y)\pi_z \\ -2\gamma\sqrt{3}(\pi_x + i\pi_y)\pi_z & 0 & 0 & 0 \\ 0 & 2\gamma\sqrt{3}(\pi_x + i\pi_y)\pi_z & 0 & 0 \end{array} \right),
$$

where $\gamma$ is the Fermi velocity and $s\kappa = \gamma_1 - \gamma_2$ is the Landau level number.
where $\pi = p + (e/c)A$ is the kinetic momentum operator, $c$ is the light velocity, $A$ is the vector potential of the external magnetic field, and $s = eB/\hbar c$. $\gamma_1$, $\bar{\gamma}$, and $\kappa$ are the effective mass parameters [1].

Hereafter we consider the case of the magnetic field is in the $z$ direction. When $k_z = 0$, the Hamiltonian is block diagonalized as $H = H_0$ and the eigenvalues can be analytically obtained just by solving the $2 \times 2$ matrix problem [10]. An interesting nontrivial contribution arises from the interband matrix elements of $H_2$. The eigenvectors of $H$ can be written as $[1,10]$

$$\psi_{l,m} = \begin{pmatrix} c_{1,\alpha}G_{l-2} \\ c_{2,\alpha}G_l \\ c_{3,\alpha}G_{l-1} \\ c_{4,\alpha}G_{l+1} \end{pmatrix},$$

(9)

in terms of the functions

$$G_l = \frac{e^{ik_xx+k_zz}}{\sqrt{L_xL_z}} \sqrt{\frac{s}{2l!\sqrt{\pi}}}H_l(t)e^{-t^2/2},$$

(10)

where $t = \sqrt{s}y - k_z/\sqrt{s}$ and $H_l(t)$ is the Hermite polynomials. The functions $G_l$ satisfy following relations in terms of $s$ and $\zeta = k_z/\sqrt{s}$:

$$(\pi_x^2 + \pi_y^2)G_l = h^2s(2l+1)G_l,$$

(11)

$$(\pi_x + i\pi_y)G_l = -h\sqrt{s}\sqrt{2(l+1)}G_{l+1},$$

(12)

$$(\pi_x - i\pi_y)G_l = -h\sqrt{s}\sqrt{2l}G_{l-1},$$

(13)

$$\pi_zG_l = h\sqrt{s}\zeta G_l.$$  

(14)

For each quantum number $l$, there are four different eigenvalues, whose degree of freedom is denoted by $\alpha = 1 \sim 4$. The coefficients $c_{1,\alpha} \sim c_{4,\alpha}$ are determined by solving numerically the $4 \times 4$ secular equation.

3. Anomalous $g$-factor

The eigenenergies of the Luttinger Hamiltonian for $\gamma_1 = 13.20$, $\bar{\gamma} = 4.92$, and $\kappa = 3.30$, which are the parameters for Ge [10], are shown in Fig. 1. Not the that the energy axis is inverted in Fig. 1, namely, the hole bands look like “electron like”. The left and right panels of Fig. 1 correspond to the heavy and light holes, respectively. A non-parabolic dispersion, which was pointed out by Wallis and Bowlden [10], is obtained for the heavy holes. This non-parabolic dispersion is due to $H_2$ and gives an unusual effective $g$-factors.

The effective $g$-factor is determined by [11]

$$g^* = \frac{E_n^\uparrow - E_n^\downarrow}{\mu_B B} = 2\frac{E_n^\uparrow - E_n^\downarrow}{e\hbar B}. \quad (15)$$

According to this definition, we firstly calculated the exact effective $g$-factor for every energy levels of the Luttinger Hamiltonian as is shown in Fig. 2 for heavy holes. We found $g^* \propto |k_z|$ for large $l$, which is consistent with the approximate theory by Yafet [11]. As discussed before, this $k_z$-dependent $g^*$ can generate nontrivial spin current.
Figure 1. Eigenenergies with respect to $\zeta = k_z / \sqrt{\kappa}$ for heavy (left) and light (right) holes under a magnetic field. The energies are measured in units of $\hbar eB/mc$. The energy axis are inverted, i.e., the hole band looks like “electron like” in this figure.

Figure 2. Effective $g$-factor for heavy holes as a function of $\zeta = k_z / \sqrt{\kappa}$.

4. Matrix elements and selection rules
In order to obtain detailed information of the conductivity, it is important to investigate the selection rules for the matrix elements of the velocity operator since the conductivity can be
calculated in terms of the matrix elements of the velocity operators as

$$
\sigma_{\mu \nu} = \frac{1}{i \omega} \left[ \Phi_{\mu \nu} ( \omega + i \delta) - \Phi_{\mu \nu} (0 + i \delta) \right], \quad (16)
$$

$$
\Phi_{\mu \nu} (i \omega \lambda) = -e^2 T \sum_{n, \alpha, \beta} \langle i | v | j \rangle \langle j | v | i \rangle \mathcal{G} (i \varepsilon_n) \mathcal{G} (i \varepsilon_n - i \lambda), \quad (17)
$$
on the basis of the Kubo formula [13, 14], where \( \mathcal{G} \) is the thermal Green’s function. The velocity operator along the field direction is given by

$$
v_z = \frac{\partial \mathcal{H}}{\hbar \partial k_z} = \frac{1}{m} \begin{pmatrix}
(\gamma_1 - 2\gamma) \pi_x & 0 & -\sqrt{3}\gamma \pi_- & 0 \\
0 & (\gamma_1 + 2\gamma) \pi_x & 0 & \sqrt{3}\gamma \pi_- \\
-\sqrt{3}\gamma \pi_+ & 0 & (\gamma_1 + 2\gamma) \pi_x & 0 \\
0 & \sqrt{3}\gamma \pi_+ & 0 & (\gamma_1 - 2\gamma) \pi_x \\
\end{pmatrix}, \quad (18)
$$

where \( \pi_\pm = \pi_x \pm i \pi_y \). It is found by using Eqs. (11)-(14) that the matrix elements for \( v_z \), \( \langle \psi_{\alpha l} | v_z | \psi_{\alpha l'} \rangle \) is finite only between \( l = l' \). (Note that the matrix elements for \( v_x \) and \( v_y \) give contribution only between \( l = l' \pm 1 \).) The result for \( v_z \) is obtained as follows:

$$
\langle \psi_{\alpha l} | v_z | \psi_{\alpha l'} \rangle = V_{\text{intra}} + V_{\text{inter}}, \quad (19)
$$

$$
V_{\text{intra}} = \left[ (c_1 c_1' + c_4 c_4') (\gamma_1 - 2\gamma) + (c_2 c_2' + c_3 c_3') (\gamma_1 + 2\gamma) \right] \frac{\hbar k_z}{m}, \quad (20)
$$

$$
V_{\text{inter}} = \left[ (c_1 c_3 + c_3 c_1') \sqrt{1-T} - (c_2 c_4 + c_4 c_2') \sqrt{1+T} \right] \frac{\hbar \gamma \sqrt{6} s}{m}, \quad (21)
$$

where we omitted the subscript \( \alpha \) of \( c_1 \). \( V_{\text{intra}} \) originates from the diagonal elements of Eq. (18) or \( \mathcal{H}_1 \), so it corresponds to the intraband transition. \( V_{\text{inter}} \) originates from the off-diagonal elements of Eq. (18) or \( \mathcal{H}_2 \), so it corresponds to the interband transition between light and heavy hole bands. The intraband contribution is proportional to \( \hbar k_z/m \), which is just the velocity at \( B = 0 \), and independent form the magnetic field. This is the trivial contribution: the normal longitudinal magnetoconductivity does not depend on the magnetic field. On the other hand, the interband contribution is proportional to \( \gamma \sqrt{B} \). This magnetic field dependent term, whose origin is the same as the anomalous \( g \)-factor, would give a nontrivial contribution: the spin current proposed in the first section of this paper.

When we measure the dc magnetoconductivity, we obtain the summation of intra- and interband contributions, and we cannot distinguish between the two contributions. However, it is interesting to compare the intensity of the interband contribution to the intraband one as

$$
\left| \frac{V_{\text{inter}}}{V_{\text{intra}}} \right|^2 = \left| \frac{(c_1 c_3 + c_3 c_1') \sqrt{1-T} - (c_2 c_4 + c_4 c_2') \sqrt{1+T}}{(c_1 c_1' + c_4 c_4') (\gamma_1 - 2\gamma) + (c_2 c_2' + c_3 c_3') (\gamma_1 + 2\gamma)} \right|^2 \frac{6\gamma^2 s}{k_z^2} \sim \frac{\gamma^2}{\gamma_1^2 \zeta^2}. \quad (22)
$$

The interband contributions will increase as the magnetic field is increased. The interband contribution should be amplified in the ac magnetoconductivity with an appropriate frequency. Also, if we can obtain a material that has large \( \gamma/\gamma_1 \), we will have the larger interband contributions. This will be achieved by using heavier elements such as Sn and Pb.
5. Conclusion

We have proposed the nontrivial contribution appears in the magnetoconductivity of the Luttinger Hamiltonian by investigating the effective $g$-factor and the selection rules for the matrix elements of the longitudinal velocity operator. The effective $g$-factor for every Landau levels of the Luttinger Hamiltonian is exactly obtained for the first time. It was confirmed that, for heavy hole band, $g^* \propto |k_z|$ for large quantum numbers of Landau levels, which was originally pointed out by approximate theory of Yafet [11]. This anomalous $g$-factor is due to the interband effect of the magnetic field between the light and heavy hole bands.

We have proposed that the $k_z$-dependent $g$-factor can generate a nontrivial spin current in the longitudinal magnetoconductivity. To confirm this idea, we have investigated the selection rules for the matrix elements of the longitudinal velocity operator. We found a nontrivial contribution actually appears in the longitudinal magnetoconductivity also due to the interband effect between light and heavy hole bands. This nontrivial contribution will generate the spin current, which can be amplified by the magnetic field or the external light with an appropriate frequency.

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