The effective field theory of \((2 + 1)\)-dimensional topological insulator in the presence of Rashba spin–orbit interaction

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Abstract

\((2 + 1)\)-dimensional topological insulator described by the Kane–Mele model in the presence of Rashba spin–orbit interaction is considered. The effective action of the external fields coupled to electromagnetic and spin degrees of freedom is accomplished within this model. The Hamiltonian methods are adopted to provide the coefficients appearing in the action. It is demonstrated straightforwardly that the coefficients of the Chern–Simons terms are given by the first Chern number attained through the related non-Abelian Berry gauge field. The effective theory which we obtain is in accord with the existence of the spin Hall phase where the value of the spin Hall conductivity is very close to the quantized one.

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(Some figures may appear in colour only in the online journal)

1. Introduction

The Kane–Mele model of monolayer graphene [1] provides a formulation of the \((2+1)\)-dimensional time reversal invariant topological insulator. In this new topological phase of matter which is also known as the quantum spin Hall insulator, the bulk is insulating but there exist topologically protected gapless edge states. Charge carriers of graphene are effectively massless Dirac-like fermions at the Dirac points in the low energy and long wavelength regime. Kane and Mele explored properties of these electrons in the presence of intrinsic as well as Rashba spin–orbit interactions. In the Kane–Mele model when only the intrinsic spin–orbit coupling is considered, two copies of the Haldane model [2] are combined to procure a quantized spin Hall conductivity. In [1] it was argued that when both the intrinsic and Rashba coupling terms are present, although the spin Hall conductivity is not quantized it has a value which slightly differs from the quantized one. Indeed, this is confirmed in [3] by numerical methods. Because of weak intrinsic spin–orbit coupling strength, the spin Hall
phases in graphene is not experimentally realizable [4, 5]. However, there are some recent proposals of synthesizing new materials which possess the honeycomb structure of graphene with a large spin–orbit gap. For instance in [6] a system of ultracold gas of potassium atoms was shown to provide an analogue of graphene. There is also silicene which is a monolayer of Si atoms possessing the same lattice structure as graphene [7], whose low energy effective Hamiltonian is the same as that with the Kane–Mele model [8]. Realization of molecular graphene [9] was another exiting achievement. In fact, in [10] it was argued that molecular graphene can be used to realize the Kane–Mele quantum spin Hall model. In this construction, the presence of the Rashba spin–orbit coupling term is essential, it cannot be switched off. Hence, it would be very helpful to have a better understanding of the main features of the Kane–Mele model in the presence of Rashba interaction. We approach this problem from an effective action point of view.

Possessing effective field theory of the external fields coupled to charge and spin degrees of freedom is an efficient tool to reveal the general predictions of topological insulators [11]. Effective theories are insensible to the internal structure of the inspected material, yet give its response to the external fields. When only the intrinsic spin–orbit coupling term is taken into account, the effective theory of (2+1)-dimensional time reversal invariant topological insulator is well established [11, 12]. It is a topological field theory where the coefficients appearing in the action are related to the first Chern numbers of the constituting Dirac-like Hamiltonians. If one introduces only the external electromagnetic gauge field, the effective Lagrange density is given by the Chern–Simons term whose coefficient vanishes. This was expected because of the fact that the underlying model is time reversal invariant in contrast to the Chern–Simons action which changes sign under this symmetry. However, one can also couple an external field to the third component of spin which combines with the electromagnetic field to procure a non-vanishing effective action whose coefficient is the quantized spin Hall conductivity [13]. In the presence of Rashba interaction the third component of spin is not conserved, nevertheless one can still deal with the spin Hall conductivity whose presence indicates the spin Hall phase. We would like to reveal if the expected spin Hall conductivity can be obtained from the effective action of the external electromagnetic and spin fields within the Kane–Mele model in the presence of Rashba interaction. This effective theory was studied in terms of Lagrangian methods in [14] where the relevant coefficients were derived at the first order in the Rashba coupling constant. We prefer to derive the effective action of the external fields coupled to charge and spin degrees of freedom of the fully fledged Kane–Mele model within Hamiltonian methods where the link between the coefficients taking part in the effective theory and topological Chern numbers can be discovered straightforwardly.

In the next section, we first recall how one constructs the effective theory when only the intrinsic spin–orbit coupling term is present. Then we will discuss how to extend this method to obtain the effective action for the fully fledged Kane–Mele model. The main difficulty shows up in the calculation of the coefficients which are defined in terms of Green functions. We would like to employ the Foldy–Wouthuysen transformation to obtain the one particle Green function for the Dirac-like Hamiltonian of the Kane–Mele model. In section 3, we explicitly construct the related Green functions and calculate the coefficients explicitly. Because of employing the Foldy–Wouthuysen transformation we straightforwardly construct the non-Abelian Berry gauge field and demonstrate that the coefficients of Chern–Simons terms are given by the first Chern number. Calculation of the other coefficient is cumbersome. Some details of this lengthy calculation are reported in the appendix. The results which we obtained are in agreement with the existence of the spin Hall phase where the spin Hall conductivity possesses approximately the quantized value. In the last section, we discuss the results which we obtained as well as a possible relation to another approach.
2. Effective field theory

Graphene has a honeycomb lattice structure based on two sublattices namely A and B. At the two inequivalent Dirac points $K$ and $K'$ of the Brillouin zone, valence and conduction bands touch each other. Around these points in the low energy and long wavelength limit, charge carriers effectively obey the free, massless Dirac-like Hamiltonian

$$H_0 = \sigma_i \tau_z p_i + \sigma_i p_i,$$

where we set the effective velocity of electrons equal to 1, $v_F = 1$. The Pauli spin matrices $\sigma_{x,y,z}$ act on the states of the sublattices $A$, $B$, and $\tau_z = \text{diag}(1, -1)$ denotes the Dirac points $K, K'$. We suppress the direct products between different spaces. In [1], Kane and Mele suggested to generate a mass gap by the intrinsic spin–orbit coupling term

$$H_{SO} = \Delta_{SO} \sigma_z \tau_z \sigma_z.$$

They also considered the Rashba spin–orbit interaction term

$$H_R = \lambda_R (\sigma_x \tau_y \sigma_y - \sigma_y \tau_x \sigma_x),$$

where the constant parameter $\lambda_R$ is experimentally tunable. The Pauli spin matrices $s_{x,y,z}$ correspond to the spin degrees of freedom of electrons. Hence, the Hamiltonian of the Kane–Mele model including intrinsic as well as Rashba spin–orbit interactions is

$$H = H_0 + H_{SO} + H_R.$$  

(2.1)

For $\lambda_R = 0$, the third component of spin, $s_z$, which can be labeled by $\uparrow \downarrow$ is conserved. Thus, the spin current can directly be defined by $j^{\text{spin}} = j^\uparrow - j^\downarrow$. It leads to the quantized spin Hall conductivity $\sigma_{SH} = 1/2\pi$, in the $e = 1, \hbar = 1$ units. This spin current can also be derived from the action, $\mu, \nu, \rho = 0, 1, 2$,

$$S_z = \frac{1}{2\pi} \int d^3 x \epsilon^{\mu\nu\rho} \Omega_\mu \partial_\nu A_\rho,$$

(2.2)

where $A_\mu$ and $\Omega_\mu$ are the external fields associated with the electromagnetic and the spin currents [13]. As we will discuss above, (2.2) results as the effective action obtained by integrating out the fermionic fields in the path integral of the field theory described by the following Lagrangian density of the Kane–Mele model for $\lambda_R = 0$,

$$\mathcal{L}_0 = \bar{\psi} \left[ \gamma^\mu \left( i \partial_\mu + A_\mu + \frac{S_z}{2} \Omega_\mu \right) - \Delta_{SO} \right] \psi.$$  

(2.3)

Here $\gamma^0 = \sigma_z s_z, \gamma^1 = i \sigma_z s_z, \gamma^2 = -i \sigma_z s_z$, and $S_z = \text{diag} (s_z, s_z, s_z)$. We would like to extend this stratagem for deriving the spin Hall conductivity to the fully fledged Kane–Mele model given by (2.1). Although when $\lambda_R$ is nonvanishing the third component of spin does not commute with the Hamiltonian (2.1), so that the current $j^{\text{spin}}_\mu = \bar{\psi} \gamma^\mu S_z \psi / 2$ is not conserved, one can still define a spin current which is conserved in the low energy limit (for a similar approach, see [15]) and calculate the spin Hall conductivity. Indeed, Kane and Mele argued that when $\Delta_{SO} > \lambda_R$ the Hamiltonian (2.1) yields the spin Hall conductivity which slightly differs from the quantized value $1/2\pi$. This is confirmed in [3] by studying the model numerically. We approach this problem from another point of view. We would like to derive the effective field theory of external fields $A_\mu, \Omega_\mu$, considering the Kane–Mele model Lagrange density in the presence of Rashba spin–orbit interaction:

$$\mathcal{L} (\psi, \bar{\psi}, A, \Omega) = \bar{\psi} \left[ \gamma^\mu \left( i \partial_\mu + A_\mu + \frac{S_z}{2} \Omega_\mu \right) - \Delta_{SO} - \lambda_R (\sigma_x s_y - \sigma_y s_x) \right] \psi.$$  

(2.4)
In the partition function,

$$Z = \int D\psi D\bar{\psi} DA_\mu D\Omega_\mu e^{i S_{\text{eff}}},$$

we may integrate out $\psi$ and $\bar{\psi}$ to acquire the effective theory of the external fields $A_\mu$, $\Omega_\mu$:

$$\int D\psi D\bar{\psi} DA_\mu D\Omega_\mu e^{i S_{\text{eff}}} = \int DA_\mu D\Omega_\mu e^{i S_{\text{eff}}}. $$

$S_{\text{eff}}$ is defined as

$$S_{\text{eff}} [A, \Omega] = -i \ln \det \left[ i \gamma^\mu \left( \partial_\mu - i A_\mu - i \frac{\lambda}{2} \Omega_\mu \right) - \Delta_{\text{SO}} - \lambda_R (\sigma \tau_s - \sigma_s \tau) \right].$$

(2.5)

We are interested only in the following terms which (2.5) evokes in the low energy limit,

$$S_{\text{eff}} = C \int d^3 x \epsilon^{\mu\nu\rho} A_\mu \partial_\nu A_\rho + C_s \int d^3 x \epsilon^{\mu\nu\rho} \Omega_\mu \partial_\nu \Omega_\rho + C_\Omega \int d^3 x \epsilon^{\mu\nu\rho} \Omega_\mu \partial_\nu \Omega_\rho.$$ 

(2.6)

This action yields the spin current

$$j^\mu_{\text{spin}} = \frac{\delta S_{\text{eff}}}{\delta \Omega_\mu}.$$ 

It is worth mentioning that the spin current obtained from the action (2.6) is conserved $\partial_\mu j^\mu_{\text{spin}} = 0$, though the third component of spin $S_z$ does not commute with the Hamiltonian (2.1). It is a consequence of dealing with the low-energy limit where the higher order gradient terms in the expansion of (2.5) are ignored.

In the weak field approximation, the coefficients in (2.6) are given in terms of the fermion propagator $G(p)$ and its inverse $G^{-1}(p)$ by [17]

$$C = -\frac{1}{12} \epsilon^{\mu\nu\rho} \int \frac{d^3 p}{(2\pi)^3} \text{tr} [G(p) \partial_\mu G^{-1}(p) [G(p) \partial_\nu G(p) [G(p) \partial_\rho G^{-1}(p)]]].$$

(2.7)

$$C_s = -\frac{1}{12} \epsilon^{\mu\nu\rho} \int \frac{d^3 p}{(2\pi)^3} \text{tr} [S_z G(p) \partial_\mu G^{-1}(p) [G(p) \partial_\nu G(p) [G(p) \partial_\rho G^{-1}(p)]]].$$

(2.8)

$$C_\Omega = -\frac{1}{12} \epsilon^{\mu\nu\rho} \int \frac{d^3 p}{(2\pi)^3} \text{tr} [S_z G(p) \partial_\mu G^{-1}(p) [S_z G(p) \partial_\nu G(p) [G(p) \partial_\rho G^{-1}(p)]]].$$

(2.9)

where $\partial_\mu = \partial / \partial p^\mu$. For $\lambda_R = 0$, we can write $H_0 + H_{\text{SO}} = \text{diag}(H^{1+}, H^{-}, H^{1-}, H^{-})$ in terms of 2 × 2 matrices, where $\pm$ labels the Dirac points $K, K'$. One can show that the coefficients can be expressed in terms of the related first Chern numbers ([11, 12] and the references therein). In fact the coefficients of the Chern–Simons terms are given by

$$C(\lambda_R = 0) = C_\Omega(\lambda_R = 0) = (N_1^{1+} + N_1^{-} + N_1^{1-} + N_1^{-}) / 4\pi.$$ 

The related first Chern numbers were obtained to be $N_1^{1\pm} = 1/2$, $N_1^{1\pm} = -1/2$. Thereby one observes that $C(\lambda_R = 0) = C_\Omega(\lambda_R = 0) = 0$. Vanishing of these coefficients was expected due to the fact that the Kane–Mele model is time reversal invariant but the Chern–Simons terms lack this symmetry. However, the other coefficient is given by

$$C_s(\lambda_R = 0) = (N_1^{1+} + N_1^{-} - N_1^{1-} - N_1^{-}) / 4\pi = 1/2\pi.$$ 

Therefore, (2.2) occurs to be the effective action of the theory described by (2.3).

In the presence of Rashba interaction, i.e. $\lambda_R \neq 0$, the coefficients (2.7)–(2.9) were constructed within Lagrangian methods in [14] up to the first-order terms in $\lambda_R / \Delta_{\text{SO}}$. Moreover,
in [16] an effective theory for a model which is similar to the Kane–Mele model\(^1\) was constructed. The following section is devoted to the explicit calculations of these coefficients.

3. Calculation of the coefficients

To attain the one particle Green function of free Dirac field \(G(p)\), we would like to employ the Hamiltonian methods. We choose to order the direct products such that the explicit form of the Kane–Mele model Hamiltonian (2.1) becomes

\[
H = \begin{pmatrix}
\sigma_x & 0 & 0 & p_x - ip_y & 0 & 0 & 0 \\
0 & -\sigma_x & 0 & 0 & 2i\sigma_R & p_x - ip_y & 0 \\
0 & 0 & -\sigma_x & 0 & 0 & -p_x - ip_y & 2i\sigma_R \\
p_x + ip_y & 0 & 0 & -\sigma_x & 0 & 0 & 0 \\
0 & p_x + ip_y & 0 & 0 & -\sigma_x & 0 & 0 \\
0 & 0 & -2i\sigma_R & 0 & 0 & -\sigma_x & 0 \\
0 & 0 & 0 & -\sigma_x & 0 & 0 & -\sigma_x
\end{pmatrix}
\]

In terms of \(p^2 = p_x^2 + p_y^2\), the eigenvalues of (3.1) are calculated to be

\[
\begin{align*}
E_1 &= E_2 = \lambda_R + \sqrt{(\sigma_x - \lambda_R)^2 + p^2}, \\
E_3 &= E_4 = -\lambda_R + \sqrt{(\sigma_x + \lambda_R)^2 + p^2}, \\
E_5 &= E_6 = \lambda_R - \sqrt{(\sigma_x - \lambda_R)^2 + p^2}, \\
E_7 &= E_8 = -\lambda_R - \sqrt{(\sigma_x + \lambda_R)^2 + p^2}.
\end{align*}
\]

\(G(p)\) can be acquired by means of the Foldy–Wouthuysen unitary transformation \(U\) which is defined to satisfy

\[
U H U^\dagger = \text{diag}(E_1, \ldots, E_8) \equiv \sum_{M=1}^8 E_M I^M.
\]

Here \(I^M\) is the matrix whose elements vanish other than \((I^M)_{MM} = 1\). The eigenfunctions corresponding to the energy eigenvalues (3.2) can be employed to establish the unitary matrix \(U\) which diagonalizes the Hamiltonian (3.1), as follows,

\[
U = \begin{pmatrix}
0 & 0 & -iF_1 & 0 & 0 & -iF_1 & 0 & 0 \\
0 & 0 & 0 & -iF_2 & 0 & 0 & -iF_2 & 0 \\
iF_1 & 0 & 0 & 0 & -iF_1 & 0 & 0 & -iF_1 \\
0 & iF_2 & 0 & 0 & 0 & -iF_2 & 0 & 0 \\
iF_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & iF_2 & 0 & 0 & 0 & 0 & 0 & 0 \\
-iF_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
iF_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\]

\(^1\) In [16], it was claimed that the model considered is equivalent to the Kane–Mele model (2.1), because of only employing another representation of the gamma matrices given by \(\gamma^\nu = \sigma_i \gamma_{KM}^\nu\), where \(\gamma_{KM}^\nu\) are the gamma matrices of the Kane–Mele model. However, they adopted the definition \(\gamma^0 = \sigma_0\) which leads to the erroneous result \(\gamma_{KM}^0 = 1\). In fact, multiplying the Pauli matrices by \(\sigma_0\) yields an equivalent set of matrices if one also takes into account the identity matrix \(1_{\nu}\), i.e. multiplying the set of matrices \((\sigma_+, \sigma_-, 1_{\nu}, \sigma_\nu)\) by \(\sigma_0\) one gets the equivalent set of matrices \((-\sigma_-, \sigma_+, 1_{\nu}, \sigma_\nu).\)
The normalization factors are given by
\[ F_{2m-1} = \sqrt{\frac{(\Delta_{SO} - E_m)^2}{2((\Delta_{SO} - E_m)^2 + p^2)}}, \quad F_{2m} = \sqrt{\frac{p^2}{2((\Delta_{SO} - E_m)^2 + p^2)}}; \quad m = 1, 2, 3, 4. \]

(3.5)

Observe that they satisfy
\[ F_{2m-1}^2 + F_{2m}^2 = \frac{1}{2}. \]

(3.6)

Inverting the unitary transformation (3.3), we can retrieve the Hamiltonian (3.1) in the form
\[ H = \sum_{M=1}^{8} E_M p^M, \]
where we introduced \( p^M = U^\dagger p U \). Obviously \( p^M \) are projection operators:
\[ \sum_{M=1}^{8} p^M = 1, \quad p^M p^N = \delta^{MN} p^N. \]

Now, one can construct the Green function \( G(p) \) and its inverse \( G^{-1}(p) \) as
\[ G(p) = \sum_{M=1}^{8} \frac{p^M}{w - E_M}, \quad G^{-1}(p) = w - \sum_{M=1}^{8} E_M p^M, \]
where \( p^\mu = (w, p_a); \quad a = 1, 2. \) Note that the derivatives of the inverse Green function \( G^{-1}(p) \) obey
\[ \frac{\partial G^{-1}(p)}{\partial w} = 1, \quad \frac{\partial G^{-1}(p)}{\partial p_a} = -\sum_{M=1}^{8} \left( \frac{p_a}{E_M} p^M + E_M \partial_a p^M \right). \]

(3.8)

To proceed, we would like to perform the \( w \) integrations in (2.7)–(2.9). This requires that the energies \( E_M, \quad M = 1, \ldots, 8 \), are arranged to be definitely positive or negative. We restrict the values of the coupling constant to \( \Delta_{SO} > 2 \lambda_R \), so that we can divide the spectrum as \( E_\alpha, \quad \alpha = 1, 2, 3, 4 \), which are positive and \( E_i, \quad i = 5, 6, 7, 8 \), which are negative. Note that in the limit \( \lambda_R \to 0 \), the eigenvalues \( E_{1,2} \) and \( E_{3,4} \) (similarly \( E_{5,6} \) and \( E_{7,8} \)) approach each other. In the following we adopt the conventions: \( \alpha, \beta, \gamma = 1, \ldots, 4; \quad i, j, k = 5, \ldots, 8; \quad M, N = 1, \ldots, 8 \); and \( a, b = 1, 2 \).

3.1. Calculation of \( C \) and \( C_\Omega \)

The winding number (2.7) can be written as
\[ C = -\frac{1}{4} \epsilon^{ab} \int \frac{d^2 p}{(2\pi)^2} \frac{d w}{w} \text{tr}[G^2(p)\partial_\alpha G^{-1}(p)G(p)\partial_\beta G^{-1}(p)]]. \]

(3.9)

The repeating \( a \) and \( b \) indices are summed over. Employing the Green function (3.7) and the derivatives of its inverse given in (3.8), one can show that the terms explicitly linear and quadratic in \( p_a \) vanish directly and the rest after performing the \( w \) integration lead to
\[ C = -\frac{i}{16\pi^2} \epsilon^{ab} \int d^2 p \text{tr} \left\{ \sum_{\alpha, \beta, i} \frac{E_{\beta} P^\alpha}{E_a - E_i} (\partial_\alpha P^\alpha \partial_\beta P^\beta - \partial_\alpha P^\beta \partial_\beta P^\alpha) \right. \]
\[ \left. + \sum_{\alpha, i, j} \frac{E_{i} P^\alpha}{E_a - E_i} (\partial_\alpha P^\beta \partial_\beta P^j - \partial_\alpha P^j \partial_\beta P^\beta) \right\}. \]
The terms other than $\alpha = \beta$ and $i = j$ do not contribute, hence one obtains
\[
C = -\frac{i}{8\pi^2} \varepsilon^{ab} \sum_{a,b,i,j} d^3p \text{tr} \left\{ \frac{E_a}{E_a - E_i} F^a_{\alpha} \partial_\alpha P^\alpha + \frac{E_i}{E_a - E_i} P^a_{\alpha} \partial_\alpha F^\alpha \right\}. \tag{3.10}
\]

Recalling that $P^M = U^\dagger P^M U$, (3.10) can be expressed in the form
\[
C = \frac{i}{8\pi^2} \varepsilon^{ab} \sum_{a,b,i,j} d^3p \text{tr} \left\{ F^a_{\alpha} F^b_{\beta} \right\}, \tag{3.11}
\]
where we introduced $A^U_a = iU \partial_\alpha U^\dagger$. Because of being a pure gauge field its curvature identically vanishes. However, we can construct the Berry gauge field through the projection of the $A^U_a$ to the positive energy states [18] by
\[
A^B_a = i \sum_{a,\beta} F^a_{\alpha} \partial_\alpha U^\dagger U^\beta,
\]
whose field strength,
\[
F^B_{ab} = \partial_a A^B_b - \partial_b A^B_a - i [A^B_a, A^B_b].
\]
does not vanish in general. The first Chern number is defined in terms of the Berry curvature as
\[
N_1 = \frac{1}{4\pi} \int d^3p \varepsilon^{ab} \text{tr} F^B_{ab}. \tag{3.12}
\]
The topological numbers (3.9) and (3.12) are connected to each other by
\[
C = \frac{N_1}{4\pi}
\]
This relation can be accomplished by observing that, due to the identity $\sum_i I^i = 1 - \sum_a I^a$, one can express (3.11) as
\[
C = -\frac{i}{8\pi^2} \varepsilon^{ab} \sum_a d^3p \text{tr} \left\{ F^a_{\alpha} \partial_\alpha U^\dagger U^\alpha U^\dagger U^\beta \right\} + \frac{i}{8\pi^2} \varepsilon^{ab} \sum_{a,\beta} d^3p \text{tr} \left\{ F^a_{\alpha} \partial_\alpha U^\dagger U^\alpha U^\beta U^\beta \right\}. \tag{3.13}
\]

Having attained the relation between the Chern number (3.12) and the winding number (3.9), the next step is to calculate the coefficient $C$ explicitly. In a straightforward manner, (3.13) can be written as
\[
C = \frac{i}{8\pi^2} \varepsilon^{ab} \int \text{tr} \left\{ \sum_a F^a_{\alpha} \partial_\alpha U^\dagger U^\alpha U^\beta - \sum_{a,\beta} F^a_{\alpha} \partial_\alpha U^\dagger U^\alpha U^\beta \right\}. \tag{3.14}
\]

After performing the trace operation and making use of (3.4), the first term vanishes:
\[
\partial_\alpha U_{21} \partial_\alpha U^*_{21} + 2 \partial_\alpha U_{22} \partial_\alpha U^*_{22} + \partial_\alpha U_{41} \partial_\alpha U^*_{41} + 2 \partial_\alpha U_{42} \partial_\alpha U^*_{42} = 0.
\]

On the other hand, the second term in (3.14) yields
\[
\varepsilon^{ab} \left( \left\{ P^1_{11} + P^1_{14} \right\} \left( \partial_\alpha U_{21} \partial_\alpha U^*_{21} + \partial_\alpha U_{41} \partial_\alpha U^*_{41} \right) + \left\{ P^1_{12} \right\} \left( \partial_\alpha U_{22} \partial_\alpha U^*_{22} + \partial_\alpha U_{42} \partial_\alpha U^*_{42} \right) \right) + 2i \left\{ P^1_{15} + P^1_{16} \right\} \left( \partial_\alpha U_{25} \partial_\alpha U^*_{25} + \partial_\alpha U_{45} \partial_\alpha U^*_{45} \right) + \left\{ 4P^1_{22} \partial_\alpha U_{22} \partial_\alpha U^*_{22} + 4P^1_{25} \partial_\alpha U_{25} \partial_\alpha U^*_{25} \right\}. \tag{3.15}
\]

In terms of the polar coordinates
\[
p = \sqrt{p_x^2 + p_y^2}, \quad \theta = \arctan \frac{p_y}{p_x}, \tag{3.16}
\]
one can demonstrate that (3.15) vanishes as
\[
\left[ \frac{4i}{p} (F_2^2 \partial_\rho F_2^2 + F_4^2 \partial_\rho F_4^2) - \frac{8i}{p} (F_2^3 \partial_\rho F_2^3 + F_4^3 \partial_\rho F_4^3) \right] = 0.
\]

In these calculations we have utilized the explicit forms of Green functions obtained from the Kane–Mele model. However, the properties of Green functions, which led us to conclude that the coefficient \( C \) vanishes, are extendable to any Dirac-like theory whose energy spectrum possesses particle–hole symmetry.

One of the benefits of using Hamiltonian methods is the fact that the coefficients corresponding to the subspaces labeled by \( \tau \), \( \epsilon = \pm 1 \) and \( s = \uparrow \downarrow \) can be calculated explicitly. In fact, they yield the Chern numbers
\[
N_1^{\uparrow \downarrow} = 1/2, \quad N_1^{\uparrow \downarrow} = -1/2.
\]

The coefficient \( C_\Omega \) (2.9) can be demonstrated to be equal to \( C (2.7) \): Observe that
\[
S_i H (\lambda_R) S_i = H (\lambda_R).
\]

This interchanges the positive and negative energy eigenvalues within themselves:
\[
E \leftrightarrow E
\]
and
\[
E \leftrightarrow E
\]
They can be expressed as
\[
\int d^2 p \text{tr} \left\{ S_i \left( \frac{E_i P^\alpha \partial_\lambda P^\alpha}{(w - E_i)^2 (w - E_i)} - \frac{E_i P^\alpha \partial_\lambda P^\alpha}{(w - E_i)^2 (w - E_i)} \right) E_M \partial_\lambda P^M \right\},
\]
\[
\int d^2 p \text{tr} \left\{ S_i \left( \frac{E_i P^\alpha \partial_\lambda P^\alpha}{(w - E_i)^2 (w - E_i)} - \frac{E_i P^\alpha \partial_\lambda P^\alpha}{(w - E_i)^2 (w - E_i)} \right) E_M \partial_\lambda P^M \right\}.
\]

Now we can integrate over \( w \) and find that they acquire the same form:
\[
C_s^{(1)} = C_s^{(2)} = -\frac{i}{48 \pi^2} \sum_{a,i,M} \int d^2 p \text{tr} \left\{ S_i \left( \frac{E_i P^\alpha \partial_\lambda P^\alpha}{(w - E_i)^2 (w - E_i)} - \frac{E_i P^\alpha \partial_\lambda P^\alpha}{(w - E_i)^2 (w - E_i)} \right) E_M \partial_\lambda P^M \right\}.
\]

They can be expressed as
\[
C_s^{(1)} = C_s^{(2)} = -\frac{i}{48 \pi^2} \sum_{a,i,M} \int d^2 p \text{tr} \left\{ \left( (E_i - E_M) P^M S_i P^\alpha T^i + (E_i - E_M) P^M S_i P^\alpha T^i \right) \right\}.
\]
where we defined $Z^M = e^{iM\partial_0 U} \bar{U}\partial_i U$. However, due to the fact that $[\mathcal{S}_c, P^M] \neq 0$, the third constituent of (3.17) yields

$$C^{(3)}_i = -\frac{\epsilon_{ib}}{12} \sum_{L,M\neq N} \int \frac{d^3 p}{(2\pi)^3} \text{tr} \left\{ \frac{E_N - E_M) P^L S^i P^M}{(\omega - E_M)(\omega - E_N)} (E_L \partial_p P^N \partial_p E + E_N \partial_p P^N \partial_p P^N) \right\}.$$  

By performing the $w$ integration we get

$$C^{(3)}_i = -\frac{i}{48\pi^2} \int d^3 p \text{tr} \left\{ P_i^{S7} (\mathcal{T}^1 + \mathcal{T}^2) + P_i^{P8} (\mathcal{T}^2 + \mathcal{T}^4) - P_i^{I3} (\mathcal{T}^5 + \mathcal{T}^7) - P_i^{P4} (\mathcal{T}^6 + \mathcal{T}^8) \right\}$$

$$+ P_i^{E3} (E_5 - E_3)/(E_5 - E_3)^2) - E_5/(E_5 - E_3) + P_i^{E4} (E_6 - E_4)/(E_6 - E_4)^2) - E_6/(E_6 - E_4)$$

$$+ P_i^{E5} (E_7 - E_5)/(E_7 - E_5)^2) - E_7/(E_7 - E_5) + P_i^{E6} (E_8 - E_6)/(E_8 - E_6)^2) - E_8/(E_8 - E_6) \right\}.$$

(3.19)

where we introduced $P^{MN} = P^M S^N + P^N S^M$. Combining (3.19) with (3.18) we obtain $C_i$ as it is presented in the appendix. One finally obtains

$$C_i = \frac{2}{3\pi^4} \int dp$$

$$\times \left\{ F_{E1}^2 F_{E1}^2 \left[ -3E_1 E_3 - 3E_3^2 + 3(E_5 + E_7)^2 + E_5^2 + E_7^2 \right] \frac{\partial F_i^2}{(\Delta_S - E_1)^2} + 1 \leftrightarrow 3 \right\}$$

$$- F_{E1}^2 F_{E1}^2 \left[ -3E_1 E_3 - 3E_3^2 + 3(E_5 + E_7)^2 + E_5^2 + E_7^2 \right] \frac{\partial F_i^2}{(\Delta_S - E_1)^2} + 5 \leftrightarrow 7 \right\}$$

$$+ F_{E1}^2 F_{E1}^2 \left[ (E_1 - E_3)^2 \frac{\partial F_i^2}{(\Delta_S - E_1)^2} - (E_1 - E_3)^2 \frac{\partial F_i^2}{(\Delta_S - E_1)^2} \right]$$

$$+ F_{E1}^2 F_{E1}^2 \left[ (E_1 - E_3)^2 \frac{\partial F_i^2}{(\Delta_S - E_1)^2} - (E_1 - E_3)^2 \frac{\partial F_i^2}{(\Delta_S - E_1)^2} \right]$$

(3.20)

where $M \Leftrightarrow N$ denotes the term which arises from the former entry by interchanging $M$ and $N$. Although we could not analytically solve the integral in (3.20), numerical calculations are in accord with the result

$$C_i = R(\infty) - R(0),$$

(3.21)

where $R(p)$ is deduced to be

$$R(p) = \frac{1}{6\pi} \int \frac{\Delta_S - \lambda_R}{\sqrt{(\Delta_S - \lambda_R)^2 + p^2}} + \frac{\Delta_S + \lambda_R}{\sqrt{(\Delta_S + \lambda_R)^2 + p^2}}$$

$$- \frac{\Delta_S}{2\lambda_R} \tanh^{-1} \left[ \frac{1 + \frac{p^2}{(\Delta_S - \lambda_R)^2}}{\frac{\lambda_R}{(\Delta_S + \lambda_R)^2}} \right] + \frac{\Delta_S}{2\lambda_R} \tanh^{-1} \left[ \frac{1 + \frac{p^2}{(\Delta_S + \lambda_R)^2}}{\frac{\lambda_R}{(\Delta_S - \lambda_R)^2}} \right].$$

(3.22)

In the limit $p \rightarrow \infty$ (3.22) vanishes, but its $p \rightarrow 0$ limit depends on the ratio of the coupling constants $\Delta_S$ and $\lambda_R$ as

$$\lim_{p \rightarrow 0} R(p) = \frac{1}{3\pi} \left[ 1 + \frac{\Delta_S}{4\lambda_R} \ln \left( \frac{\Delta_S + \lambda_R}{\Delta_S - \lambda_R} \right) \right].$$

For diverse values of the coupling constants satisfying $\Delta_S > 2\lambda_R$, $C_i$ occurs to be in the range between $0.506/\pi$ and $0.500/\pi$. For example, we find $C_i = 0.506/\pi$ for $\frac{\Delta_S}{\lambda_R} = 3$ and $C_i = 0.502/\pi$ for $\frac{\Delta_S}{\lambda_R} = 5$. As we plotted in figure 1, for $\frac{\Delta_S}{\lambda_R} > 5$, (3.21) has values closer to $C_i = 1/2\pi$ which is the exact result when $\Delta_S \gg \lambda_R$. 

9
4. Discussions

Response of the system (2.4) to the field $\Omega_\mu$, provided by the effective action (2.6), is

$$j^\mu_{\text{spin}} = C^s e^{\mu\nu\rho} \partial_\nu A_\rho,$$

where $C^s \approx e/2\pi$. We do not deal with the quantum corrections to the $BF$-type action (2.6). Otherwise, in the expansion of (2.5) we need to consider the higher gradient terms which we ignored in the low-energy limit. The spatial component of the spin current can be interpreted in terms of the spin Hall conductivity $\sigma_{\text{SH}}$ and the electric field $E_a = \partial_\alpha A_\alpha - \partial_\alpha A_\alpha$ as

$$j^a_{\text{spin}} = \sigma_{\text{SH}} \epsilon_{abc} E_c.$$

Thus, we can conclude that for the Kane–Mele model in the presence of Rashba interaction (2.4) it has approximately the quantized value

$$\sigma_{\text{SH}} = C^s \approx \frac{1}{2\pi},$$

(4.1)

for $\Delta_{\text{SO}} > 2\lambda_R$.

Within the Kane–Mele model in the presence of Rashba interaction, (2.4), a realization of the $(2 + 1)$-dimensional spin Hall phase in a certain range of values of the interaction parameters, $\Delta_{\text{SO}}, \lambda_R$, was suggested in [10]. In this molecular graphene construction to achieve quantum spin Hall phase a suitable set of values was given by $\Delta_{\text{SO}} = 0.145$ eV and $\lambda_R = 0.04$ eV. In fact, adopting these values, our numerical calculation produces the result $\sigma_{\text{SH}} \approx 1/2\pi$.

Moreover, response of the Kane–Mele model (2.4) to the external electromagnetic gauge field $A_\mu$, can be derived from the effective action (2.6) as

$$j^\mu_{\text{charge}} = \frac{\delta S_{\text{eff}}}{\delta A_\mu}.$$

We have shown that the coefficient of the Chern–Simons term, $C$, vanishes, so that the charge current furnished by the effective action is

$$j^\mu_{\text{charge}} \approx \frac{1}{2\pi} e^{\mu\nu\rho} \partial_\nu \Omega_\rho.$$

(4.2)
In [11], it was demonstrated that (4.2) is the fundamental response equation for the quantum spin Hall effect.

To consider the spin Hall phase, a topological invariant spin Chern number was introduced in [19]. The definition of [19] relies on the fact that one can project eigenstates of a gapped Hamiltonian to up and down sectors of the spin operator $S_z$, even if it does not commute with the related Hamiltonian. In [20], this definition was adopted to calculate the spin Chern numbers $N_{\pm \uparrow \downarrow}^{SC}$ for the Kane–Mele model in the presence of Rashba interaction. As we have already noted, $\pm$ and $\uparrow \downarrow$ label the Dirac points and the $S_z$ eigenvalues. They obtained

\[ N_{\pm \uparrow}^{SC} = K_{\pm \uparrow}(\infty) - K_{\pm \uparrow}(0) = \frac{1}{2}, \]
\[ N_{\pm \downarrow}^{SC} = K_{\pm \downarrow}(\infty) - K_{\pm \downarrow}(0) = -\frac{1}{2}, \]

where

\[ K_{\pm \uparrow}(p) = -K_{\pm \downarrow}(p) = F_2(p)F_4(p), \]
\[ K_{- \uparrow}(p) = -K_{- \downarrow}(p) = F_6(p)F_8(p). \]  

(4.3)

Now, the ‘total spin Chern number’ relevant to obtain the spin current can be defined as follows:

\[ N^{SC} = N_{\uparrow \downarrow}^{SC} + N_{- \uparrow \downarrow}^{SC} - N_{- \downarrow \uparrow}^{SC} - N_{- \downarrow \downarrow}^{SC} = 2. \]  

(4.4)

Although the momentum dependence of $R(p)$ and $K(p)$ given in (3.22) and (4.3) is not the same, the numerical results (4.1) and (4.4) suggest that

\[ \sigma_{SH} \approx \frac{1}{4\pi} N^{SC}. \]

Obviously, this suggested relation between the coefficient of effective action $C_s$ and the ‘total spin Chern number’ $N^{SC}$ needs further clarifications.

We only dealt with non-interacting electrons. When electron–electron interactions on the honeycomb lattice are introduced in terms of the Hubbard model, the third component of spin is still a good quantum number in the absence of Rashba spin–orbit interactions [21, 22]. Because of being a many-body system, it is not evident how to incorporate Hubbard interactions into the field theory of the Kane–Mele model. For the mean-field decoupled Hubbard interactions, the electron–electron interaction results in shifting the intrinsic spin–orbit coupling $\Delta_{SO}$ with a constant related to the Hubbard onsite energy $U$, due to the properties of the Hubbard model ($\Delta_{SO} = 0, \lambda_R = 0$) [21]. Hence, when we switch on Rashba spin–orbit interactions, the related field theory for the mean-field decoupled Hubbard interactions will be described by a Lagrangian density similar to (2.4) up to some constants. On the other hand, in [23] a field theory of the Kane–Mele model with Hubbard interactions was proposed in terms of some auxiliary fields which are associated with spin gauge field components. Although this formalism reproduces the original model on-shell, how one should take into account the loop contributions of the auxiliary fields is not clear.

We demonstrated that the response of the quantum spin Hall insulator in the presence of Rashba interaction can be obtained from the effective action of the external electromagnetic and spin fields (2.6). Therefore, the materials analogous to graphene yield predictions which are independent of their detailed structure as far as the underlying Hamiltonian is given by the Kane–Mele model. Their response can be studied within the $BF$-type topological field theory of the external fields.

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Appendix

Calculation of the coefficient $C_s$ is straightforward, though it is very cumbersome. Here we would like to present the essential steps of the calculation of $C_s$. First of all, one can observe that (3.18) can be expressed in terms of $P^{MN} = P^M S_N + P^N S_M$, so that it can be amalgamated with (3.19) to write $C_s$ as:

$$C_s = -\frac{1}{48\pi^2} \int d^2 p \text{tr} \left[ p^5 \left( 1 + \frac{E_1 - E_2}{E_1 - E_5} + \frac{E_1 - E_5}{E_1 - E_7} \right) T^1 + \left( 1 + \frac{E_4 - E_5}{E_3 - E_5} + \frac{E_3 - E_5}{E_3 - E_7} \right) T^3 \right]$$

$$+ p^{12} \left[ \left( 1 + \frac{E_2 - E_6}{E_2 - E_5} + \frac{E_2 - E_9}{E_2 - E_7} \right) T^1 + \left( 1 + \frac{E_4 - E_8}{E_4 - E_6} + \frac{E_4 - E_6}{E_4 - E_8} \right) T^2 \right]$$

$$- p^{13} \left[ \left( 1 + \frac{E_3 - E_4}{E_3 - E_1} + \frac{E_3 - E_1}{E_3 - E_5} \right) T^1 + \left( 1 + \frac{E_7 - E_3}{E_7 - E_1} + \frac{E_7 - E_1}{E_7 - E_3} \right) T^3 \right]$$

$$- p^{24} \left[ \left( 1 + \frac{E_6 - E_2}{E_6 - E_5} + \frac{E_6 - E_5}{E_6 - E_7} \right) T^1 + \left( 1 + \frac{E_8 - E_2}{E_8 - E_6} + \frac{E_8 - E_6}{E_8 - E_2} \right) T^2 \right]$$

$$+ p^{15} \left[ \left( 1 + \frac{E_1 - E_3}{E_1 - E_5} + \frac{E_1 - E_5}{E_1 - E_7} \right) T^1 + \left( 1 + \frac{E_5 - E_3}{E_5 - E_1} + \frac{E_5 - E_1}{E_5 - E_3} \right) T^3 \right]$$

$$+ p^{16} \left[ \left( 1 + \frac{E_2 - E_4}{E_2 - E_6} + \frac{E_2 - E_6}{E_2 - E_4} \right) T^1 + \left( 1 + \frac{E_4 - E_2}{E_4 - E_6} + \frac{E_4 - E_6}{E_4 - E_2} \right) T^3 \right]$$

$$+ p^{17} \left[ \left( 1 + \frac{E_3 - E_1}{E_3 - E_5} + \frac{E_3 - E_5}{E_3 - E_7} \right) T^1 + \left( 1 + \frac{E_5 - E_3}{E_5 - E_1} + \frac{E_5 - E_1}{E_5 - E_3} \right) T^3 \right]$$

$$+ p^{28} \left[ \left( 1 + \frac{E_4 - E_2}{E_4 - E_6} + \frac{E_4 - E_6}{E_4 - E_2} \right) T^1 + \left( 1 + \frac{E_6 - E_4}{E_6 - E_2} + \frac{E_6 - E_2}{E_6 - E_4} \right) T^3 \right] .$$

Making use of the polar coordinates (3.16) and the definitions (3.5), one can show that it can be written in the form:

$$C_s = -\frac{1}{12\pi^2} \int d^2 p \left[ \frac{F_2^2 F_3^2 p A(5, 7)}{(\Delta_{SO} - E_1)(\Delta_{SO} - E_2)(\Delta_{SO} - E_7)} \right]$$

$$\times \left( 1 + \frac{E_1 - E_2}{E_1 - E_5} + \frac{E_1 - E_5}{E_1 - E_7} \right) (E_5 - E_1) \delta p F_1^3$$

$$- \frac{F_2^2 F_3^2 C(6, 8)}{p(\Delta_{SO} - E_2)} \left( 1 + \frac{E_2 - E_4}{E_2 - E_6} + \frac{E_2 - E_6}{E_2 - E_4} \right) (E_6 - E_2) \delta p F_2^2$$

$$+ \frac{F_2^2 F_3^2 p A(5, 7)}{(\Delta_{SO} - E_3)(\Delta_{SO} - E_5)(\Delta_{SO} - E_7)} \left( 1 + \frac{E_4 - E_5}{E_4 - E_6} + \frac{E_4 - E_6}{E_4 - E_5} \right) (E_5 - E_4) \delta p F_3^2$$

$$- \frac{F_2^2 F_3^2 C(6, 8)}{p(\Delta_{SO} - E_4)} \left( 1 + \frac{E_4 - E_6}{E_4 - E_8} + \frac{E_4 - E_8}{E_4 - E_6} \right) (E_8 - E_4) \delta p F_4^2$$

$$+ \frac{F_2^2 F_3^2 p A(1, 3)}{(\Delta_{SO} - E_5)(\Delta_{SO} - E_6)(\Delta_{SO} - E_3)} \left( 1 + \frac{E_6 - E_5}{E_6 - E_3} + \frac{E_6 - E_3}{E_6 - E_5} \right) (E_5 - E_6) \delta p F_2^2$$

$$- \frac{F_2^2 F_3^2 C(2, 4)}{p(\Delta_{SO} - E_6)} \left( 1 + \frac{E_6 - E_4}{E_6 - E_8} + \frac{E_6 - E_8}{E_6 - E_4} \right) (E_8 - E_6) \delta p F_4^2$$

$$+ \frac{F_2^2 F_3^2 p A(1, 3)}{(\Delta_{SO} - E_1)(\Delta_{SO} - E_2)(\Delta_{SO} - E_7)} \left( 1 + \frac{E_2 - E_1}{E_2 - E_5} + \frac{E_2 - E_5}{E_2 - E_7} \right) (E_7 - E_2) \delta p F_1^2$$

$$- \frac{F_2^2 F_3^2 C(2, 4)}{p(\Delta_{SO} - E_1)} \left( 1 + \frac{E_1 - E_3}{E_1 - E_6} + \frac{E_1 - E_6}{E_1 - E_3} \right) (E_6 - E_1) \delta p F_1^2$$
where we defined
\[ A(m, n) = 2 \left[ 1 + \frac{p^2}{(\Delta SO - E_m)(\Delta SO - E_n)} \right], \]
\[ C(m, n) = 2 \left[ 1 + \frac{(\Delta SO - E_m)(\Delta SO - E_n)}{p^2} \right]. \]

Expressing \( A(m, n) \) and \( C(m, n) \) in terms of the normalization factors (3.5), it can further be simplified as
\[ C_i = -\frac{1}{6\pi^2} \int d^3 p \frac{F_i F_j + F_j F_k) F_k F_j}{p(\Delta SO - E_1)} \left[ 1 + \frac{E_1 - E_2}{E_2 - E_1} \right] \left( 1 + \frac{E_4 - E_5}{E_5 - E_4} + \frac{E_6 - E_5}{E_5 - E_6} \right) \left( E_5 - E_1 \right) \partial_p F_2^2 \]
\[ F_i F_j + F_j F_k) F_k F_j}{p(\Delta SO - E_2)} \left( 1 + \frac{E_2 - E_6}{E_6 - E_2} \right) \left( E_6 - E_2 \right) \partial_p F_2^2 \]
\[ F_i F_j + F_j F_k) F_k F_j}{p(\Delta SO - E_3)} \left( 1 + \frac{E_3 - E_5}{E_5 - E_3} + \frac{E_6 - E_5}{E_5 - E_6} \right) \left( E_6 - E_3 \right) \partial_p F_3^2 \]
\[ F_i F_j + F_j F_k) F_k F_j}{p(\Delta SO - E_4)} \left( 1 + \frac{E_4 - E_5}{E_5 - E_4} + \frac{E_6 - E_5}{E_5 - E_6} \right) \left( E_6 - E_4 \right) \partial_p F_4^2 \]
\[ F_i F_j + F_j F_k) F_k F_j}{p(\Delta SO - E_5)} \left( 1 + \frac{E_5 - E_3}{E_3 - E_5} + \frac{E_6 - E_5}{E_5 - E_6} \right) \left( E_6 - E_5 \right) \partial_p F_5^2 \]
\[ F_i F_j + F_j F_k) F_k F_j}{p(\Delta SO - E_6)} \left( 1 + \frac{E_6 - E_4}{E_4 - E_6} \right) \left( E_6 - E_4 \right) \partial_p F_6^2 \]
\[ F_i F_j + F_j F_k) F_k F_j}{p(\Delta SO - E_7)} \left( 1 + \frac{E_7 - E_3}{E_3 - E_7} \right) \left( E_7 - E_3 \right) \partial_p F_7^2 \]
\[ F_i F_j + F_j F_k) F_k F_j}{p(\Delta SO - E_8)} \left( 1 + \frac{E_8 - E_4}{E_4 - E_8} \right) \left( E_8 - E_4 \right) \partial_p F_8^2 \]
\[ F_i F_j + F_j F_k) F_k F_j}{p(\Delta SO - E_9)} \left( 1 + \frac{E_9 - E_3}{E_3 - E_9} \right) \left( E_9 - E_3 \right) \partial_p F_9^2 \]
\[ F_i F_j + F_j F_k) F_k F_j}{p(\Delta SO - E_{10})} \left( 1 + \frac{E_{10} - E_3}{E_3 - E_{10}} \right) \left( E_{10} - E_3 \right) \partial_p F_{10}^2 \]
\[ F_i F_j + F_j F_k) F_k F_j}{p(\Delta SO - E_{11})} \left( 1 + \frac{E_{11} - E_3}{E_3 - E_{11}} \right) \left( E_{11} - E_3 \right) \partial_p F_{11}^2 \]
\[ F_i F_j + F_j F_k) F_k F_j}{p(\Delta SO - E_{12})} \left( 1 + \frac{E_{12} - E_3}{E_3 - E_{12}} \right) \left( E_{12} - E_3 \right) \partial_p F_{12}^2 \]
\[ F_i F_j + F_j F_k) F_k F_j}{p(\Delta SO - E_{13})} \left( 1 + \frac{E_{13} - E_3}{E_3 - E_{13}} \right) \left( E_{13} - E_3 \right) \partial_p F_{13}^2 \]
\[ F_i F_j + F_j F_k) F_k F_j}{p(\Delta SO - E_{14})} \left( 1 + \frac{E_{14} - E_3}{E_3 - E_{14}} \right) \left( E_{14} - E_3 \right) \partial_p F_{14}^2 \]
Finally, by making use of relations like

\[
1 - \frac{F_3 F_5}{F_4 F_6} = \frac{E_1 - E_3}{E_1 - \Delta_{SO}},
\]

(3.20) is accomplished.

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