Quantum Atmospherics for Materials Diagnosis

Qing-Dong Jiang[1], Frank Wilczek[1234]
[1]*Department of Physics, Stockholm University, Stockholm SE-106 91 Sweden*
[2]*Center for Theoretical Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139 USA*
[3]*T. D. Lee Institute, and Wilczek Quantum Center, Department of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai 200240, China*
[4]*Department of Physics and Origins Project, Arizona State University, Tempe AZ 25287 USA*

Symmetry breaking states of matter can transmit symmetry breaking to nearby atoms or molecular complexes, perturbing their spectra. We calculate one such effect, involving the "axion electrodynamics" relevant to topological insulators, quantitatively. We provide an operator framework whereby effects of this kind can be analyzed systematically, qualitatively, and discuss possible experimental implications.

Introduction: Over the past few decades physicists have come to appreciate the importance of increasingly subtle forms of symmetry breaking in materials, often connected with topology and entanglement. Many new states of matter characterized by such "hidden" symmetry breaking have been proposed theoretically, but concrete, unambiguous experimental manifestations have been relatively sparse. Many of the proposed states violate some combination of the discrete symmetries P, T. This opens up the possibility of unusual polarizabilities, generalizing the familiar dielectric and para- or diamagnetic response parameters ϵ, μ. Those polarizabilities can support novel electromagnetic effects, which reflect the discrete symmetry breaking directly. Here we will discuss one such effect in quantitative detail, and then provide a general framework which supports systematic qualitative discussion.

Atmosphere from Axion Electrodynamics: Consider a material whose interaction with the electromagnetic field contains an action term

$$\int d^3x dt\, \chi_M(x)\, \Delta\mathcal{L}_{\text{axion}} \;=\; \int d^3x dt\, \chi_M(x)\, \kappa\, \vec{E}\cdot\vec{B}\,, \tag{1}$$

where $\chi_M(x)$ is the characteristic function of the material. This sort of interaction was contemplated in [1], and it is realized in topological insulators [2–4], with $\kappa = j\alpha$, where j is an odd integer. Since $\vec{E}\cdot\vec{B}$ is a total derivative, it does not affect the bulk equations of motion. But when the spatial region occupied by the material is bounded, surface terms arise. Specifically, if the plane $z = 0$ forms an upper boundary, we will have a surface action

$$\int d^3x dt\, \chi_M(x)\, \kappa\, \vec{E}\cdot\vec{B}$$
$$\rightarrow \frac{\kappa}{2}\int dx\, dy\, dt\, \epsilon^{3\alpha\beta\gamma} A_\alpha(x,y,0,t)\partial_\beta A_\gamma(x,y,0,t). \tag{2}$$

This gives us a two-photon vertex which violates the discrete symmetries P, T, while preserving PT. Quantum fluctuations involving this vertex will produce a sort of P, T violating atmosphere above the material. (See Figure 1.) The atmosphere induces new kinds of "Casimir" forces on bodies near the material [5–7]. It also induces new kinds of effective interactions within atoms or molecular centers, which effect their spectra. Such interactions are especially interesting, because in favorable cases the spectra can be measured quite accurately, thus plausibly rendering small symmetry-violating effects accessible.

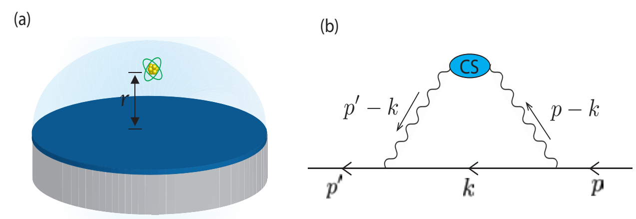

FIG. 1. (a) Illustration of quantum atmosphere induced by a Chern-Simon surface. The blue layer corresponds to the top surface described by a Chern-Simon term at $z = 0$. Due to quantum fluctuation, time-reversal symmetry breaking effect will be transmitted to the nearby atom at the distance r from the surface. (b) Feynman diagram involving Chern-Simon vortex.

Let us analyze the most basic case, that is the interaction of an electron. By symmetry and dimension counting, the first-order effective P, T violating interaction with an electron, at a distance r from a planar boundary, will take the form

$$\mathcal{L}_{\text{int.}} \;\sim\; \frac{\alpha\kappa}{mr^2}\,\hat{n}\cdot\vec{s}, \tag{3}$$

where $m, \vec{s}$ are the electron's mass and spin, and $r, \hat{n}$ are the distance and normal to the plane. Expressed using fundamental units only, as in the quoted form for topological insulators, we find the dimensional estimate

$$\mathcal{L}_{\text{int.}} \;\sim\; \frac{\alpha^2}{mr^2}\,\hat{n}\cdot\vec{s} \approx \left(\frac{10\,\text{nm.}}{r}\right)^2 \frac{e\hat{n}\cdot s}{m}\, 10 \text{ gauss.} \tag{4}$$

Here we have expressed the atmospheric Zeeman-like interaction in a form which allows ready comparison with the Zeeman splitting induced by a magnetic field strength. Taken at face value, this is comfortably within the estimated sensitivity of magnetometry based on NV centers [8] – by many orders of magnitude (but see below). Note however that we do not generate true magnetic flux, so that SQUID detectors are not suitable (but see below).

We can check this estimate by explicit calculation, according to the Feynman digram of Figure 1. We find [9]

$$V(r) \ = \ \frac{\kappa e^2}{128\pi^2}\,\frac{1}{mr^2}\,\sigma_3 \ \rightarrow \frac{j\alpha^2}{32\pi}\,\frac{1}{mr^2}\,\sigma_3 \qquad (5)$$

One might attempt to generalize this calculation to particles which possess an anomalous magnetic moment (e.g., atomic nuclei), but one encounters an ultraviolet divergence. This is not a physical contradiction, because both anomalous magnetic moments and (especially) our assumed action Eqn. (1) will have form-factors which provide cut-offs. Also for this reason, our estimate Eqn. (4) and the result of our calculation Eqn. (5) should be regarded as encouraging, but not dispositive.

We can also consider the effect of applying an external electric field. Importantly, this does not in itself introduce T violation. If we apply an electric field parallel to the boundary plane, we induce a surface Hall-like current. A planar current sheet produces a spatially constant (true) magnetic field, which will be aligned (or anti-aligned) with the applied electric field. To maximize the induced field while avoiding cancellations between contributions from opposite sides of the material, we should use samples with effective surfaces whose linear dimensions are large compared to the distance to the test atom or complex, but small compared to the separation between surfaces. If we apply an electric field perpendicular to the boundary plane, it induces a surface magnetic charge, and thus again a magnetic field aligned or anti-aligned with the applied electric field, and in the same sense. The magnitudes of the magnetic fields, for moderate values of the applied electric field, can be quite substantial:

$$B \ \sim \ \kappa E \ \rightarrow \ \alpha E \ \approx \ 10^{-1}\,\text{gauss}\left(\frac{E}{10^4\,\frac{\text{V}}{\text{cm.}}}\right) \qquad (6)$$

where the progression from general to particular is as previously. These induced currents and fields were anticipated in [1]; here we are adding some context on their connection with symmetry and their possible experimental accessibility. They are a much more conservative application of the effective theory.

Apart from spontaneous P, T symmetry breaking in materials, we may also have intrinsic violation. A generic signature of such violation is the existence of particles having both elementary magnetic dipole moments and (small) elementary electric dipole moments. A material containing a density ρ of such particles will, in the presence of an applied electric field at temperature T, contain a density $\rho g_e \vec{E}/T$ of aligned spins, and hence an energy density $\left(g_m g_e/T\right)\rho\vec{E}\cdot\vec{B}$. Thus, we identify an alternative source of our action Eqn. (1), with $\kappa = \rho g_m g_e/T$. In this model, it is transparently clear why a normal electric field, by inducing a magnetic dipole density, yields a surface magnetic charge density. Some possible experimental arrangements to probe intrinsic symmetry breaking effects of this kind were discussed in [10] from a very different point of view. Numerically, we have

$$\begin{aligned} B &\sim \rho g_m g_e E/T \\ &\sim \left(\frac{\rho}{\frac{10^{22}}{\text{cm}^3}}\right)\frac{g_e}{10^{-26}\text{e cm}}\,\frac{E}{10^6\,\frac{\text{V}}{\text{cm}}}\,\frac{10^{-3}\text{K}}{T}\,10^{-12}\text{gauss} \end{aligned} \qquad (7)$$

where we have inserted the electron gyromagnetic moment, aggressive reference values of the parameters, and a reference value of the electric dipole moment comparable to current limits. The resulting magnetic field is well within advertised sensitivities [8]. It would be good to revisit this issue in the light of modern technology.

Operator Analysis of Polarizabilities: In constructing effective theories of electromagnetism in condensed matter, there are few principles we can apply *a priori*. Nevertheless, when plausible assumptions and approximations give us tractable theories which contain few parameters, those theories can be very useful in organizing data and planning experiments. For our purposes, it is instructive to recall that textbooks of electromagnetism commonly introduce just two material-dependent parameters, ϵ and μ, to describe a wide range of observed behaviors. They can be considered as coefficients in the Maxwell action

$$\begin{aligned} &\int d^3x dt\, \chi_M(x)\, \Delta\mathcal{L}_{\text{Maxwell}} \\ &= \ \int d^3x dt\, \chi_M(x)\, \frac{\epsilon}{2}\vec{E}^2 \ - \ \frac{1}{2\mu}\vec{B}^2\,. \end{aligned} \qquad (8)$$

These are the possible terms which satisfy four sorts of conditions:

1. They are local in space and time, containing only products of fields at the same space-time point.
2. They are invariant under many symmetries: time and space translation, rotation, gauge.
3. They are quadratic in fields and of lowest possible order (i.e., zero) in space and time gradients.
4. They are invariant under P and T symmetry.

Eqn. (1) is an additional term we can bring in if we drop the last of those conditions. Aside from symmetry, is also commonly ignored because it does not contribute to the bulk equations of motion, but as we have seen that reason is superficial.

The third condition is practical rather than fundamental. Indeed, terms containing higher powers of fields are the meat and potatoes of nonlinear optics [12]. But in many circumstances it is appropriate to ignore nonlinear effects. Also, it is often appropriate to consider external and effective fields which vary smoothly in space in time. With those ideas in mind, we can get a nice inventory of the possible terms which are quadratic in fields and of lowest order in space and time gradients while consistent with 1.-3. and displaying different P, T characters. We arrive at the following candidate Lagrangian densities:

- *P even, T even*: Maxwell terms, Eqn. (8)

$$\begin{aligned} \mathcal{O}_E &= \vec{E}^2 \\ \mathcal{O}_B &= \vec{B}^2 \end{aligned} \tag{9}$$

- *P odd, T odd*: axion electrodynamics, Eqn. (1)

$$\mathcal{O}_a = \vec{E}\cdot\vec{B} \tag{10}$$

- *P even, T odd*:

$$\begin{aligned} \mathcal{O}_1 &= \frac{\partial \vec{E}}{\partial t}\cdot\vec{E} = \frac{\partial}{\partial t}\frac{1}{2}\vec{E}^2 \\ \mathcal{O}_2 &= \frac{\partial \vec{B}}{\partial t}\cdot\vec{B} = \frac{\partial}{\partial t}\frac{1}{2}\vec{B}^2 \\ \mathcal{O}_3 &= \left[(\nabla\times\vec{E})\cdot\vec{B}\right] \\ \mathcal{O}_4 &= (\nabla\times\vec{B})\cdot\vec{E} = \mathcal{O}_3 - \nabla\cdot(\vec{E}\times\vec{B}) \end{aligned} \tag{11}$$

- *P odd, T even*:

$$\begin{aligned} \mathcal{O}_5 &= \left[(\nabla\times\vec{E})\cdot\vec{E}\right] \\ \mathcal{O}_6 &= (\nabla\times\vec{B})\cdot\vec{B} \\ \mathcal{O}_7 &= \frac{\partial \vec{E}}{\partial t}\cdot\vec{B} \\ \mathcal{O}_8 &= \frac{\partial \vec{B}}{\partial t}\cdot\vec{E} = \frac{\partial}{\partial t}(\vec{B}\cdot\vec{E}) - \mathcal{O}_7 \end{aligned} \tag{12}$$

The bracketed terms are redundant, since the Faraday relation $\nabla\times\vec{E} = -\frac{\partial B}{\partial t}$ holds identically, when one expresses the fields in terms of potentials. Terms which are total time derivatives do not contribute to the equations of motion or to surface times, while terms which are total space divergences give boundary actions. Thus in the P even, T odd case we find only a boundary action, corresponding to $\mathcal{O}_4$, while in the P odd, T even case we get two terms, corresponding to $\mathcal{O}_6$ and $\mathcal{O}_7-\mathcal{O}_8$, which affect bulk behavior. These considerations can guide the design of experiments. For example, to search for a P violating but T invariant atmosphere (and thus, to probe for states of matter with those symmetries) we might first exclude an emergent $\hat{n}\cdot\vec{s}$ interaction in a planar geometry, and then look for an emergent $\hat{n}_1\cdot(\hat{n}_2\times\vec{s})$ interaction in a more complex geometry, involving two characteristic directions. Upon applying a time-dependent electric field, we may look for an atmospheric magnetic field whose direction changes according to whether the magnitude of $\vec{E}$ is increasing or decreasing. That behavior derives from $\mathcal{O}_7$.

Note that if we work directly at the level of polarizabilities, rather than actions, we can define contributions corresponding to all eight cases, and also two independent "axion" terms. Thus for example we might write

$$\begin{aligned} \vec{D} &= c_e\vec{E} + c_{a1}\vec{B} + c_1\frac{\partial\vec{E}}{\partial t} + c_4\nabla\times\vec{B} + c_5\nabla\times\vec{E} + c_8\frac{\partial\vec{B}}{\partial t} \\ \vec{H} &= c_b\vec{B} + c_{a2}\vec{E} + c_2\frac{\partial\vec{B}}{\partial t} + c_3\nabla\times\vec{E} + c_6\nabla\times\vec{B} + c_7\frac{\partial\vec{E}}{\partial t}\,. \end{aligned} \tag{13}$$

After applying the Faraday relation, we have ten independent terms, including the two conventional ones. The more restrictive Lagrangian approach seems more principled, however.

Materials that contain chiral molecules can violate P while conserving T intrinsically; indeed, many such so-called gyrotropic materials are well known [13]. A possibility for more subtle, spontaneous breaking of this class, which still preserves macroscopic rotation and translation symmetry, could be a non-vanishing correlation of the type $\langle\vec{j}\cdot\vec{s}\rangle \neq 0$ between microscopic current and and spin densities which are themselves uncorrelated ($\langle\vec{j}\rangle = \langle\vec{s}\rangle = 0$). Similarly, a non-vanishing correlation of the type $\langle\vec{j}\cdot\vec{\pi}\rangle \neq 0$ between microscopic current and polarization densities which are themselves uncorrelated exhibits P even, T odd spontaneous breaking; while a non-vanishing correlation $\langle\vec{s}\cdot\vec{\pi}\rangle \neq 0$ is odd under both P and T, but even under PT, as we have mentioned before implicitly.

Summary: We have discussed how quantum fluctuations, in the presence of a material, produce a kind of atmosphere which can affect the spectra of nearby atoms. The atmosphere can be probed to diagnose properties of the material, and in particular its symmetry. We have calculated one effect of this kind, by taking the effective theory based on axion electrodynamics at face value, and found a result that is very large compared to expected experimental sensitivities. The atmosphere can be influenced in a calculable way by external fields. We displayed an operator framework in which to discuss these issues systematically, and classified the simplest non-trivial possibilities under stated, broad assumptions. Our assumptions could be relaxed, for instance to allow crystalline asymmetries, at the cost of bringing in more operators. The operator analysis suggests how to probe symmetry-breaking atmospheres experimentally, and to parameterize their properties.

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Calculation of the Feynman diagram in the main text

Q.-D. Jiang and F. Wilczek

I. TWO-PHOTON EXCHANGE FEYNMAN DIAGRAM

Consider an electron moving at a distance r above a Chern-Simon (CS) surface at $z = 0$. The action has the following form

$$S = \int d^4x \, \left\{ \bar{\psi} \left[\gamma^\mu (p_\mu - eA_\mu) - m \right] \psi - \frac{1}{4} F_{\mu\nu} F^{\mu\nu} \right\} + \int d^4x \, \epsilon^{\alpha\beta\gamma 3} A_\alpha \partial_\beta A_\gamma \, \delta(x_3). \tag{1}$$

We separate the whole action into free part and interaction part, i.e., $S = S_0 + S_I$, where

$$S_0 = \int d^4x \, \left\{ \bar{\psi} \left[\gamma^\mu p_\mu - m \right] \psi - \frac{1}{4} F_{\mu\nu} F^{\mu\nu} \right\}; \tag{2}$$

$$S_I = S_I^a + S_I^b = \int d^4x \, \bar{\psi} \left(-e\gamma^\mu A_\mu \right) \psi + \int d^4x \, \epsilon^{\alpha\beta\gamma 3} A_\alpha \partial_\beta A_\gamma \, \delta(x_3). \tag{3}$$

Note that S_I^a and S_I^b, respectively, represent electron-photon vortex and CS vortex.

Now, we can consider the generating function

$$Z = \frac{\int D[\bar{\psi}, \psi] D[A] \, e^{iS_0 + iS_I}}{\int D[\bar{\psi}, \psi] D[A] \, e^{iS_0}} = \frac{\int D[\bar{\psi}, \psi] D[A] \, e^{iS_0} \left[1 + iS_I + \frac{1}{2}(iS_I)^2 + \frac{1}{3!}(iS_I)^3 + ... \right]}{\int D[\bar{\psi}, \psi] D[A] \, e^{iS_0}} \tag{4}$$

So the lowest order contribution from the CS plate is a two-photon process: (two electron-photon vortices and one CS vortex)

$$Z = \frac{\int D[\bar{\psi}, \psi] D[A] \, e^{iS_0} \left[\frac{1}{2}(i \, S_I^a)^2 (i \, S_I^b) \right]}{\int D[\bar{\psi}, \psi] D[A] \, e^{iS_0}}. \tag{5}$$

The relevant Feynman diagram [see the Figure 1] describe the interaction between the electron and Chern-Simon term can be calculated via

$$M = \int d^4x \int d^4w \int d^4z \; \bar{\psi}(z) \left(-ie\gamma^\mu \right) D_{\mu\alpha}(z - x) \, G(z - w) \left(i\partial_\beta \right) D_{\rho\delta}(x - w) \, \delta(x_3) \epsilon^{\alpha\beta\rho 3} \left(-ie\gamma^\delta \right) \psi(w) \tag{6}$$

where G and D correspond to Feynman propagators of electron and photon, respectively.

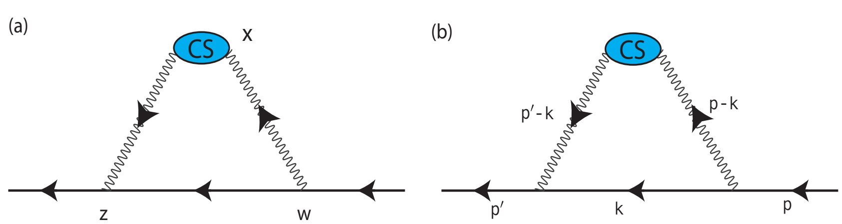

Figure 1: The Feynman diagrams in real space (a) and in momentum space (b).

Substitute the Fourier transformation of the Feynman propagators

$$D_{\mu\alpha}(z-x) = \int \frac{d^4k'}{(2\pi)^4} \frac{(-i)g_{\mu\alpha}}{k'^2 + i\epsilon} e^{-ik'(z-x)} \tag{7}$$

$$D_{\rho\delta}(x-w) = \int \frac{d^4k''}{(2\pi)^4} \frac{(-i)g_{\rho\delta}}{k''^2 + i\epsilon} e^{-ik''(x-w)} \tag{8}$$

$$G(z-w) = \int \frac{d^4k}{(2\pi)^4} \frac{i}{\gamma^\mu k_\mu - m + i\epsilon} e^{-ik(z-w)} \tag{9}$$

into the above expression Eqn. (6), and one can obtain:

$$\begin{aligned}
M =& \int d^4x \int d^4w \int d^4z\ \delta(x_3) \times \bar{u}(p') e^{ip'z} (ie\gamma^\mu) \\
& \int \frac{d^4k'}{(2\pi)^4} D_{\mu\alpha}(k') e^{-ik'(z-x)} \times (i\partial_\beta) \int \frac{d^4k''}{(2\pi)^4} D_{\rho\delta}(k'') e^{-ik''(x-w)} \epsilon^{\alpha\beta\rho 3} \times \int \frac{d^4k}{(2\pi)^4} G(k) e^{-ik(z-w)}\ e^{-ipw} (ie\gamma^\delta) u(p) \\
=& \bar{u}(p')(ie\gamma^\mu) \int dx_0 dx_1 dx_2 dx_3 \int dw_0 dw_1 dw_2 dw_3 \int dz_0 dz_1 dz_2 dz_3\ \delta(x_3) \times \\
& \int \frac{d^4k}{(2\pi)^4} \int \frac{d^4k'}{(2\pi)^4} \int \frac{d^4k''}{(2\pi)^4} \left[D_{\mu\alpha}(k') \times (k''_\beta) \times D_{\rho\delta}(k'') \right] \epsilon^{\alpha\beta\rho 3} G(k) (ie\gamma^\delta) e^{i(k'-k'')x} e^{i(k''+k-p)w} e^{-i(k+k'-p')z} u(p) \\
=& \frac{1}{2\pi} \bar{u}(p')(ie\gamma^\mu) \int d^4k \int d^4k' \int d^4k'' \left[D_{\mu\alpha}(k') \times (k''_\beta) \times D_{\rho\delta}(k'') \right] \epsilon^{\alpha\beta\rho 3} G(k)(ie\gamma^\delta) \times \\
& \delta(k'-k'')_{0,1,2}\ \delta(k'+k-p')\ \delta(k''+k-p) u(p) \\
=& \frac{1}{2\pi}\ \bar{u}(p')\, (ie\gamma^\mu) \int d^4k\, \delta(p'-p)_{0,1,2} \left[D_{\mu\alpha}(p'-k) \times (p-k)_\beta \times D_{\rho\delta}(p-k) \right] \epsilon^{\alpha\beta\rho 3} G(k)(ie\gamma^\delta) \times\ u(p)
\end{aligned} \tag{10}$$

In the Feynman gauge, photon's propagator is diagonal. So the scattering amplitude is

$$\begin{aligned}
M =& \frac{1}{2\pi}\ \delta(p'-p)_{0,1,2}\ \bar{u}(p')(ie\gamma^\mu) \int d^4k \times \\
& \frac{(-i)g_{\mu\mu}}{(p'-k)^2} \times \frac{(-i)g_{\rho\rho}}{(p-k)^2} \times (p-k)_\beta \times \frac{i}{\gamma^\nu k_\nu - m}\ \epsilon^{\mu\beta\rho 3} (ie\gamma^\rho)\, u(p)
\end{aligned} \tag{11}$$

We can explicitly write down all possible terms according to the value of β in the above formula.

(i) $\beta = 1$ term:

$$\begin{aligned}
M_1 =& -\frac{i}{2\pi}\, \delta(p'-p)_{0,1,2}\, \bar{u}(p')\, (e^2\gamma^0) \int d^4k \times \frac{1}{(p-k)^2} \times \frac{1}{(p'-k)^2} \times \frac{(p-k)_1}{\gamma^\nu k_\nu - m} \gamma^2 \times\ u(p) \\
& + \frac{i}{2\pi}\, \delta(p'-p)_{0,1,2}\, \bar{u}(p')\, (e^2\gamma^2) \int d^4k \times \frac{1}{(p-k)^2} \times \frac{1}{(p'-k)^2} \times \frac{(p-k)_1}{\gamma^\nu k_\nu - m} \gamma^0 \times\ u(p) \\
=& -\frac{ie^2}{2\pi}\, \delta(p'-p)_{0,1,2}\, \bar{u}(p') \times \\
& \int d^4k\, \frac{1}{(p-k)^2} \times \frac{1}{(p'-k)^2} \times \frac{\gamma^0 (p-k)_1\, (\gamma^\nu k_\nu + m)\gamma^2 - \gamma^2 (p-k)_1\, (\gamma^\nu k_\nu + m)\gamma^0}{k^2 - m^2} \times\ u(p)
\end{aligned} \tag{12}$$

(ii) $\beta = 2$ term:

$$\begin{aligned}
M_2 =& \frac{ie^2}{2\pi}\, \delta(p-p)_{0,1,2}\, \bar{u}(p') \times \\
& \int d^4k\, \frac{1}{(p-k)^2} \times \frac{1}{(p'-k)^2} \times \frac{\gamma^0 (p-k)_2\, (\gamma^\nu k_\nu + m)\gamma^1 - \gamma^1 (p-k)_2\, (\gamma^\nu k_\nu + m)\gamma^0}{k^2 - m^2} \times\ u(p)
\end{aligned} \tag{13}$$

(iii) $\beta = 0$ term:

$$M_3 = -\frac{ie^2}{2\pi}\,\delta(p'-p)_{0,1,2}\,\bar{u}(p')\times \int d^4k\,\frac{1}{(p-k)^2}\times\frac{1}{(p'-k)^2}\times\frac{\gamma^1(p-k)_0(\gamma^\nu k_\nu+m)\gamma^2-\gamma^2(p-k)_0(\gamma^\nu k_\nu+m)\gamma^1}{k^2-m^2}\times u(p) \tag{14}$$

II. CALCULATION OF THE INTEGRALS

First of all, let's perform Feynman parametrization to simplify the denominator.
Using Feynman parametrization trick $\frac{1}{ABC} = 2\int_0^1 du_1 \int_0^{u_1} du_2 \frac{1}{[u_2A+(u_1-u_2)B+(1-u_1)C]^3}$, one can obtain

$$\begin{aligned}\frac{1}{(p-k)^2}\times\frac{1}{(p'-k)^2}\times\frac{1}{k^2-m^2} &= 2\int_0^1 du_1\int_0^{u_1} du_2\frac{1}{[u_2(p-k)^2+(u_1-u_2)(p'-k)^2+(1-u_1)(k^2-m^2)]^3}\\ &= 2\int_0^1 du_1\int_0^{u_1} du_2\frac{1}{D^3}\end{aligned} \tag{15}$$

Here,

$$\begin{aligned}D =&u_2(p-k)^2+(u_1-u_2)(p'-k)^2+(1-u_1)(k^2-m^2)\\ =&u_2\left[(p-k)_0^2-(p-k)_1^2-(p-k)_2^2-(p-k)_3^2\right]+(u_1-u_2)\left[(p'-k)_0^2-(p'-k)_1^2-(p'-k)_2^2-(p'-k)_3^2\right]\\ &+(1-u_1)\left(k_0^2-k_1^2-k_2^2-k_3^2-m^2\right)\\ =&-u_2(p_3-k_3)^2+u_2(p_3'-k_3)^2+u_1\left[(p'-k)_0^2-(p'-k)_1^2-(p'-k)_2^2-(p'-k)_3^2\right]\\ &+(1-u_1)\left(k_0^2-k_1^2-k_2^2-k_3^2-m^2\right)\\ =&2u_2(p_3-p_3')k_3+u_1\left[({p_0'}^2-2p_0'k_0)-({p_1'}^2-2p_1'k_1)-({p_2'}^2-2p_2'k_2)-({p_3'}^2-2p_3'k_3)\right]\\ &+\left(k_0^2-k_1^2-k_2^2-k_3^2\right)-(1-u_1)m^2\\ =&(k_0^2-2u_1p_0'k_0)-(k_1^2-2u_1p_1'k_1)-(k_2^2-2u_1p_2'k_2)-\left[k_3^2-2u_1p_3'k_3+2u_2(p_3'-p_3)k_3\right]\\ &+u_1({p_0'}^2-{p_1'}^2-{p_2'}^2-{p_3'}^2)-(1-u_1)m^2\\ =&(k_0^2-2u_1p_0'k_0)-(k_1^2-2u_1p_1'k_1)-(k_2^2-2u_1p_2'k_2)-\left[k_3^2-2u_1p_3'k_3+2u_2(p_3'-p_3)k_3\right]\\ &+u_1m^2-(1-u_1)m^2\\ =&(k_0-u_1p_0')^2-(k_1-u_1p_1')^2-(k_2-u_1p_2')^2-\left[k_3-u_1p_3'+u_2(p_3'-p_3)\right]^2\\ &+(2u_1-1)m^2-(u_1p_0')^2+(u_1p_1')^2+(u_1p_2')^2+\left[-u_1p_3'+u_2(p_3'-p_3)\right]^2\\ =&(k_0-u_1p_0')^2-(k_1-u_1p_1')^2-(k_2-u_1p_2')^2-\left[k_3-u_1p_3'+u_2(p_3'-p_3)\right]^2\\ &+(-u_1^2+2u_1-1)m^2-u_1^2{p_3'}^2+((u_1-u_2)p_3'+u_2p_3)^2\\ =&l_0^2-l_1^2-l_2^2-l_3^2-(1-u_1)^2m^2-u_1^2{p_3'}^2+\left[-u_1p_3'+u_2(p_3'-p_3)\right]^2\\ =&l_0^2-l_1^2-l_2^2-l_3^2-T^2\end{aligned} \tag{16}$$

where $T^2 = (1-u_1)^2m^2+u_1^2{p_3'}^2-[u_1p_3'-u_2(p_3'-p_3)]^2$. We have used substitution of variables $l_0 = k_0-u_1p_0'$, $l_1 = k_1-u_1p_1'$, $l_2 = k_2-u_1p_2'$, $l_3 = k_3-u_1p_3'+u_2(p_3'-p_3)$, and on-shell condition of the external legs of electrons in Eqn. (16).

<u>Second, let's make some simplification of the numerator.</u>

The numerator in M_1 is

$$\begin{aligned}
&\gamma^0(p-k)_1\,(\gamma^\nu k_\nu+m)\gamma^2-\gamma^2(p-k)_1\,(\gamma^\nu k_\nu+m)\gamma^0\\
=&\gamma^0\gamma^2(p_1-k_1)\left[-\gamma^2(\not k+m)\gamma^2+\gamma^0(\not k+m)\gamma^0\right]\\
=&\gamma^0\gamma^1\gamma^2(\not p_1-\not k_1)\left[-\gamma^2(\not k+m)\gamma^2+\gamma^0(\not k+m)\gamma^0\right]\\
=&2\gamma^0\gamma^1\gamma^2(\not p_1-\not k_1)\left[m-\not k_1-\not k_3\right]
\end{aligned}\tag{17}$$

The numerator in M_2 is

$$\begin{aligned}
&-\left[\gamma^0(p-k)_2\,(\gamma^\nu k_\nu+m)\gamma^1-\gamma^1(p-k)_2\,(\gamma^\nu k_\nu+m)\gamma^0\right]\\
=&-\gamma^0\gamma^1\gamma^2(\not p_2-\not k_2)\left[\gamma^1(\not k+m)\gamma^1-\gamma^0(\not k+m)\gamma^0\right]\\
=&2\gamma^0\gamma^1\gamma^2(\not p_2-\not k_2)\left[m-\not k_2-\not k_3\right]
\end{aligned}\tag{18}$$

The numerator in M_3 is

$$\begin{aligned}
&\gamma^1(p-k)_0(\gamma^\nu k_\nu+m)\gamma^2-\gamma^2(p-k)_0(\gamma^\nu k_\nu+m)\gamma^1\\
=&-\gamma^0\gamma^1\gamma^2(\not p_0-\not k_0)\left[\gamma^2(\not k+m)\gamma^2+\gamma^1(\not k+m)\gamma^1\right]\\
=&2\gamma^0\gamma^1\gamma^2(\not p_0-\not k_0)\left[m-\not k_0-\not k_3\right]
\end{aligned}\tag{19}$$

If we add up M_1, M_2, M_3, the total numerator is

$$\begin{aligned}
&2m\gamma^0\gamma^1\gamma^2\left[(\not p_0-\not k_0)+(\not p_1-\not k_1)+(\not p_2-\not k_2)\right]\\
&-2\gamma^0\gamma^1\gamma^2\left[(\not p_0-\not k_0)(\not k_0+\not k_3)+(\not p_1-\not k_1)(\not k_1+\not k_3)+(\not p_2-\not k_2)(\not k_2+\not k_3)\right]
\end{aligned}\tag{20}$$

<u>Next, we regroup the numerator into four parts.</u>

a.

$$t_1=2m\gamma^0\gamma^1\gamma^2\left[(\not p_0-\not k_0)+(\not p_1-\not k_1)+(\not p_2-\not k_2)\right]\tag{21}$$

b.

$$t_2=2\gamma^0\gamma^1\gamma^2(k_0^2-k_1^2-k_2^2)\tag{22}$$

c.

$$t_3=-2\gamma^0\gamma^1\gamma^2\left[(\not p_0+\not p_1+\not p_2)\not k_3-(\not k_0+\not k_1+\not k_2)\not k_3\right]\tag{23}$$

d.

$$t_4=-2\gamma^0\gamma^1\gamma^2\left[p_0k_0-p_1k_1-p_2k_2\right]\tag{24}$$

The integral that we need to calculate becomes

$$M = -\frac{ie^2}{2\pi}\delta(p'-p)_{0,1,2} \times 2\int_0^1 du_1 \int_0^{u_1} du_2 \int d^4l \frac{t_1+t_2+t_3+t_4}{\left[l_0^2-l_1^2-l_2^2-l_3^3-T^2\right]^3}, \tag{25}$$

where $T^2 = \alpha^2 - \left[u_1 p_3' - u_2(p_3'-p_3)\right]^2$ with $\alpha^2 = (1-u_1)^2 m^2 + u_1^2 {p_3'}^2$.

In the following, we will often use the typical integral of momentum:

$$\begin{aligned} &\int d^4l \frac{1}{(l_0^2-l_1^2-l_2^2-l_3^2-T^2+i\epsilon)^3} \text{ (Wick rotation: } l_0 \to il_0) \\ &= -i\int d^4l \frac{1}{(l_0^2+l_1^2+l_2^2+l_3^2+T^2)^3} \\ &= -i2\pi^2 \int_0^\infty dl \frac{l^3}{(l^2+T^2)^3} = -i\frac{\pi^2}{2}\frac{1}{T^2} \end{aligned} \tag{26}$$

We will often use variable substitution $l_0 = k_0 - u_1 p_0'$, $l_1 = k_1 - u_1 p_1'$, $l_2 = k_2 - u_1 p_2'$, $l_3 = k_3 - u_1 p_3' + u_2(p_3' - p_3)$; and then perform Wick rotation $l_0 \mapsto il_0$ in the following context. In addition, we use the relations $p_0' = p_0$, $p_1' = p_1$, $p_2' = p_2$ due to the $\delta(p'-p)_{0,1,2}$ function in M. Now, we can calculate the following terms based on four different types of numerators.

a.

$$\begin{aligned} t_1 =& 2m\gamma^0\gamma^1\gamma^2 \left[(\not{p}_0' - \not{k}_0) + (\not{p}_1' - \not{k}_1) + (\not{p}_2' - \not{k}_2)\right] \\ &= -2m\gamma^0\gamma^1\gamma^2 \left[(\not{l}_0 + u_1\not{p}_0' - \not{p}_0') + (\not{l}_1 + u_1\not{p}_1' - \not{p}_1') + (\not{l}_2 + u_1\not{p}_2' - \not{p}_2')\right] \\ &= 2m\gamma^0\gamma^1\gamma^2(1-u_1)\left[\not{p}_0' + \not{p}_1' + \not{p}_2'\right] \text{ (dropped odd power of } l_\mu) \\ &= 2m(1-u_1)\left[\not{p}_0' + \not{p}_1' + \not{p}_2'\right]\gamma^0\gamma^1\gamma^2 \text{ (removed } \not{p}_\mu' \text{ to the front)} \\ &= 2m(1-u_1)\left[m - \not{p}_3'\right]\gamma^0\gamma^1\gamma^2 \text{ (used on-shell condition of Dirac equation } \bar{u}(p')(\not{p}'-m)=0) \\ &\approx 2m^2(1-u_1)\gamma^0\gamma^1\gamma^2 \text{ (in nonrelativistic limit } m >> p_1, p_2, p_3) \end{aligned} \tag{27}$$

b.

$$\begin{aligned} t_2 =& 2\gamma^0\gamma^1\gamma^2\left[(l_0+u_1p_0')^2 - (l_1+u_1p_1')^2 - (l_2+u_1p_2')^2\right] \\ &= 2\gamma^0\gamma^1\gamma^2\left[l_0^2 - l_1^2 - l_2^2 + u_1^2({p_0'}^2 - {p_1'}^2 - {p_2'}^2)\right] \text{ (dropped odd power of } l_\mu\text{, and Wick rotation} \to) \\ &= 2\gamma^0\gamma^1\gamma^2\left[-l_0^2 - l_1^2 - l_2^2 + u_1^2({p_0'}^2 - {p_1'}^2 - {p_2'}^2)\right] \\ &= -2\gamma^0\gamma^1\gamma^2(l_0^2+l_1^2+l_2^2) + 2\gamma^0\gamma^1\gamma^2 u_1^2\left({p_0'}^2 - {p_1'}^2 - {p_2'}^2\right) \\ &= -2\gamma^0\gamma^1\gamma^2(l_0^2+l_1^2+l_2^2) + 2\gamma^0\gamma^1\gamma^2 u_1^2\left(m^2 + {p_3'}^2\right) \end{aligned} \tag{28}$$

The first term $2\gamma^0\gamma^1\gamma^2(-l_0^2+l_1^2+l_2^2)$ contributes to the total scattering amplitude as

$$\begin{aligned}
&-\frac{ie^2}{2\pi}\delta(p'-p)_{0,1,2}\times 2\int_0^1 du_1\int_0^{u_1}du_2(-i)\int d^4l\frac{-2\gamma^0\gamma^1\gamma^2(l_0^2+l_1^2+l_2^2)}{(l_0^2+l_1^2+l_2^2+l_3^2+T^2)^3}\\
&=\frac{e^2}{\pi}\delta(p'-p)_{0,1,2}\times 2\gamma^0\gamma^1\gamma^2\int_0^1 du_1\int_0^{u_1}du_2\times\frac{3}{4}\int_0^\infty dl\,(2\pi^2)\frac{l^5}{(l^2+T^2)^3}\\
&=e^2\pi\delta(p'-p)_{0,1,2}\times\gamma^0\gamma^1\gamma^2\int_0^1 du_1\int_0^{u_1}du_2\times\frac{3}{2}\Gamma(0)\\
&=\frac{3\pi e^2}{4}\delta(p'-p)_{0,1,2}\gamma^0\gamma^1\gamma^2\Gamma(0)
\end{aligned}\tag{29}$$

This term is independent of scattering momentum, thus does not contribute to the effective potential.

Now, we can consider the second term

$$\begin{aligned}
&2\gamma^0\gamma^1\gamma^2u_1^2\left(m^2+{p_3'}^2\right)\ \text{(in non-relativistic limit)}\\
&\approx 2\gamma^0\gamma^1\gamma^2u_1^2m^2
\end{aligned}\tag{30}$$

c.

$$\begin{aligned}
t_3&=2\gamma^0\gamma^1\gamma^2\left[(\not k_0-\not p_0')+(\not k_1-\not p_1')+(\not k_2-\not p_2')\right]\not k_3\\
&=2\gamma^0\gamma^1\gamma^2\left[(\not l_0+u_1\not p_0'-\not p_0')+(\not l_1+u_1\not p_1'-\not p_1')+(\not l_2+u_1\not p_2'-\not p_2')\right]\times\left[\not l_3+u_1\not p_3'-u_2(\not p_3'-\not p_3)\right]\\
&=-2\gamma^0\gamma^1\gamma^2(1-u_1)u_1\left(\not p_0'+\not p_1'+\not p_2'\right)\not p_3'+2\gamma^0\gamma^1\gamma^2(1-u_1)u_2\left(\not p_0'+\not p_1'+\not p_2'\right)(\not p_3'-\not p_3)\\
&=-2(1-u_1)u_1\left[\gamma^1\gamma^2\gamma^3p_0'p_3'+\gamma^0\gamma^2\gamma^3p_1'p_3'-\gamma^0\gamma^1\gamma^3p_2'p_3'\right]\\
&\quad+2(1-u_1)u_2\left[\gamma^1\gamma^2\gamma^3p_0'(p_3'-p_3)+\gamma^0\gamma^2\gamma^3p_1'(p_3'-p_3)-\gamma^0\gamma^1\gamma^3p_2'(p_3'-p_3)\right]\\
&=-2(1-u_1)u_1\left[\gamma^0\gamma^2\gamma^3p_1'p_3'-\gamma^0\gamma^1\gamma^3p_2'p_3'\right]+2(1-u_1)u_2\left[\gamma^0\gamma^2\gamma^3p_1'(p_3'-p_3)-\gamma^0\gamma^1\gamma^3p_2'(p_3'-p_3)\right]\\
&=-2(1-u_1)u_1A+2(1-u_1)u_2B
\end{aligned}\tag{31}$$

If we want to calculate $\int_0^1 du_1\int_0^{u_1}du_2\,\frac{t_3}{T^2}$, we need to perform the following two integrals:

$$\int_0^{u_1}du_2\frac{u_2}{\alpha^2-\left[u_1p_3'-u_2(p_3'-p_3)\right]^2}\ \ [2(1-u_1)B]\tag{32}$$

$$\int_0^{u_1}du_2\frac{1}{\alpha^2-\left[u_1p_3'-u_2(p_3'-p_3)\right]^2}\ \ [-2(1-u_1)u_1A]\tag{33}$$

where $\alpha^2=(1-u_1)^2m^2+u_1^2{p_3'}^2$.

Because $\int_0^{u_1}du_2\frac{u_2}{\alpha^2-\left[u_1p_3'-u_2(p_3'-p_3)\right]^2}=\frac{u_1^2}{\alpha^2}\cdot\frac{p_3'}{p_3'-p_3}$, and $\int_0^{u_1}du_2\frac{1}{\alpha^2-\left[u_1p_3'-u_2(p_3'-p_3)\right]^2}=\frac{u_1}{\alpha^2}$. Then, you will find these two integrals exactly canceled with each other. So we don't need to consider the term c anymore. Note that these integrals are calculate under the assumption $p_1\,,p_2\,,p_3<<m$.

There is another way to prove the vanish of t_3 term by invoking the symmetry of the integral. With the substitution $u_2\to u_1-u_2$, the whole integral remains unchanged. So one can use the combination $\frac{1}{2}(u_2+u_1-u_2)=\frac{u_1}{2}$ to represent u_2. Remember $p_3'=-p_3$, then one can show the two terms in t_3 cancel out with each other.

d.

$$\begin{aligned} t_4 =& -2\gamma^0\gamma^1\gamma^2\left[p'_0k_0 - p'_1k_1 - p'_2k_2\right] \\ &= -2\gamma^0\gamma^1\gamma^2\left[p'_0(l_0+u_1p'_0) - p'_1(l_1+u_1p'_1) - p'_2(l_2+u_1p'_2)\right] \\ &= -2\gamma^0\gamma^1\gamma^2u_1\left({p'_0}^2 - {p'_1}^2 - {p'_2}^2\right) \\ &= -2\gamma^0\gamma^1\gamma^2u_1\left(m^2 + {p'_3}^2\right) \\ &\approx -2\gamma^0\gamma^1\gamma^2u_1m^2 \end{aligned} \tag{34}$$

Add up t_1, t_2 and t_4, and the numerator becomes

$$t_1 + t_2 + t_4 = 2m^2(1 - u_1 + u_1^2 - u_1)\gamma^0\gamma^1\gamma^2 = 2m^2(1-u_1)^2\gamma^0\gamma^1\gamma^2 \tag{35}$$

Consider $t_1 + t_2 + t_4$, we need to calculate the integral:

$$\begin{aligned} &\left[2m^2\gamma^0\gamma^1\gamma^2\right]\int_0^1 du_1\int_0^{u_1} du_2\left(-\frac{i\pi^2}{2}\right)\frac{(1-u_1)^2}{T^2} \\ &= \left[2m^2\gamma^0\gamma^1\gamma^2\right]\left(-\frac{i\pi^2}{2}\right)\int_0^1 du_1\frac{u_1(1-u_1)^2}{\alpha^2} \\ &= \left[(-i\pi^2)\gamma^0\gamma^1\gamma^2\right]\frac{m^4 - \pi m^3p'_3 - 4m^2{p'_3}^2 + 3m^2{p'_3}^2\,log(\frac{m}{p'_3})^2}{2m^4} \end{aligned} \tag{36}$$

We collect all the gradients and only care about the off-diagonal scattering amplitude, which is

$$\begin{aligned} M &= \delta(p'-p)_{0,1,2}\,\bar{u}\left(-\frac{ie^2}{2\pi}\right)\times\left[(-i\pi^2)\gamma^0\gamma^1\gamma^2\right]\left(-\frac{\pi}{2}\right)\frac{p'_3}{m}\times u \\ &= \delta(p'-p)_{0,1,2}\,\bar{u}\left(\frac{\pi^2e^2}{4}\right)\gamma^0\gamma^1\gamma^2\frac{p'_3}{m}\times u \end{aligned} \tag{37}$$

In non-relativistic limit, $u \to \left(\xi,\ \frac{\mathbf{p}\cdot\sigma}{2m}\xi\right)^T$, to the first order p'_3/m, the scattering amplitude for spin up/down electron is

$$M = \delta(p'-p)_{0,1,2}\ i\,\xi^\dagger\left(-\frac{\pi^2e^2}{4}\right)\frac{p'_3}{m}\sigma_3\,\xi \tag{38}$$

In the scattering process, the transferred momentum is $\tilde{p} = (0, 0, 0, 2p'_3)$. Fourier transform the scattering matrix, we can get the effective interaction

$$\begin{aligned} V(r) &= \frac{1}{(2\pi)^4}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} d\tilde{p}_0\,d\tilde{p}_1\,d\tilde{p}_2\ \delta(\tilde{p})_{0,1,2}\ e^{-i\tilde{p}_0x_0+i\tilde{p}_1x_1+i\tilde{p}_2x_2}\ \times 2\int_0^\infty d\tilde{p}_3\ \left(-\frac{\pi^2e^2}{4}\right)\frac{p'_3}{m}\sigma_3e^{i\tilde{p}_3r} \\ &= \frac{1}{16\pi^4}\left(-\frac{\pi^2e^2}{4}\right)\times 4\int_0^\infty dp'_3\,\frac{p'_3}{m}\,\sigma_3\,e^{2ip'_3r} \\ &= -\frac{e^2}{16\pi^2}\int_0^\infty dp'_3\,\frac{p'_3}{m}\,\sigma_3\,e^{2ip'_3r}\ (\text{Wick rotation } p'_3 \to ip'_3) \\ &= \frac{e^2}{16\pi^2}\int_0^\infty dp'_3\,\frac{p'_3}{m}\,\sigma_3\,e^{-2p'_3r} \\ &= \frac{e^2}{64\pi^2}\frac{1}{mr^2}\sigma_3 \end{aligned} \tag{39}$$

Note that, in our calculation, the coefficient before Chern-Simon term is 1. For the surface of a topological insulator, we can put the coefficient as $\frac{\kappa}{2} = \frac{j\alpha}{2}$, where j is an odd number. Thus, our final result becomes

$$\begin{aligned} V(r) &= j\frac{\kappa}{2} \times \frac{e^2}{64\pi^2}\frac{1}{mr^2}\sigma_3 \\ &= j\frac{\alpha^2}{32\pi}\frac{1}{mr^2}\sigma_3 \end{aligned} \tag{40}$$