Quantum Atmospherics for Materials Diagnosis

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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

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

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.

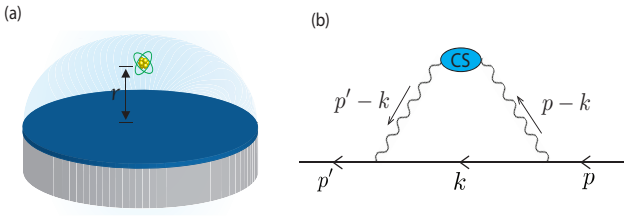


FIG. 1. (a) Illustration of quantum atmosphere induced by a Chern-Simon surface. The blue layer corresponds to the top surface described by a Chern-Simon term at $z = 0$. Due to quantum fluctuation, time-reversal symmetry breaking effect will be transmitted to the nearby atom at the distance r from the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

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

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:

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

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 $\big(g_m g_e/T\big)\rho\vec{E}\cdot\vec{B}$. 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

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

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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