A Comment On Berry Connections

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ABSTRACT: When families of quantum systems are equipped with a continuous family of Hamiltonians such that there is a gap in the common spectrum one can define a notion of a Berry connection. In this note we stress that, in general, since the Hilbert bundle defining the family of quantum systems does not come with a canonical trivialization there is in fact not a single Berry connection but rather a family of Berry connections. Two examples illustrate that this remark can have physical consequences. June 7, 2017
1. Introduction And Conclusion

In this paper we comment on a little subtlety in the definition of “Berry phases” and “Berry connections” which seems to have been overlooked in reviews such as [3, 5, 9, 33]. Put briefly: The usual discussion explains that a Berry connection depends on three pieces of data:

1. A bundle of Hilbert spaces $\pi : \mathcal{H} \rightarrow X$ over a space $X$ of control parameters.
2. A family of Hamiltonians parametrized by $X$.
3. A choice of energy cutoff defining “low energy states.”

In fact, there is a fourth piece of data that is needed in the construction: One must also choose a connection on the bundle $\mathcal{H}$. In general there are many choices for such a connection, and the choice can have physical consequences. What principles ought to be used to make this choice is an interesting question. It is part of the specification of the physical problem, and a full discussion of such principles is far beyond the scope of this letter.

In this letter the need to include the fourth piece of data is illustrated with two examples. These examples are, unfortunately, not too dramatic, but they do suffice to make the
point that the subtlety under discussion can have physical consequences. The first example resolves a minor paradox about the standard expression for electric polarizability per unit volume due to valence electrons in an insulator \cite{20, 31, 32} and is ultimately rather trivial as a physical effect. The other effect is more interesting and is associated with the formula for the “axion angle” of an insulator in \(3 + 1\) dimensions \cite{13, 14, 35}. It leads to the \(3 + 1\) dimensional version of the quantum Hall effect, explored by B. Halperin et. al. about 25 years ago \cite{18, 21}. (In fact, demanding mathematical naturalness in the formulation of the Berry connection led me on an independent path to the \(3 + 1\) dimensional QHE. But it was then pointed out to me by A. Furusaki and N. Read that the \(3 + 1\) dimensional QHE is a standard and well-known result.)

While the two examples we give here are, perhaps, uninspiring, we believe that this subtlety will play a role in many other physical examples. One such example arises in studying families of two-dimensional conformal field theories with toroidal target spaces. These naturally lead to a bundle of CFT statespaces over Narain moduli spaces. There is more than one “natural” connection on these statespaces so that any discussion of phenomena associated to Berry connections on low-lying states (e.g. the moduli themselves) will be subject to the subtlety we are discussing. Another example where we expect our considerations to play a role is in higher-dimensional \(tt^*\) geometry \cite{8}.

There is also a derivation of “the” Berry connection from integrating out heavy modes (a.k.a. fast modes) in a path integral \cite{22, 23}. The subtlety we are discussing is related to the choice of boundary conditions used for the heavy fields. \(^1\) It might be interesting to explore this approach in more detail. There should also be a parallel discussion for families of quantum systems with noncommutative control parameters, as described in \cite{26}, and again we leave that for the future.

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2. Definition Of Berry Connections

2.1 Hilbert Bundles

Let \(X\) be a topological space. \(X\) is to be thought of as a space of control parameters, parametrizing some family of quantum systems. For simplicity we will take \(X\) to be a

\(^1\)I thank A. Kapustin for a discussion on this point.
connected space. Let
\[ \pi : \mathcal{H} \to X \]
be a Hilbert bundle. This means the fibers \( \pi^{-1}(x) := \mathcal{H}_x \) are Hilbert spaces and over a suitable open cover \( \{U_\alpha\} \) there are isomorphisms \( \varphi_\alpha : \pi^{-1}(U_\alpha) \cong U_\alpha \times \mathcal{H}_0 \), where \( \mathcal{H}_0 \) is a fixed Hilbert space, and the transition functions \( \varphi_\beta \circ \varphi_\alpha^{-1} \) on patch overlaps \( U_\alpha \cap U_\beta \) are continuous maps to the unitary group of \( \mathcal{H}_0 \), in a suitable topology. (The details of the topology we use can be found in Appendix D of [15].) A crucial point for this note will be the distinction between a \textit{trivializable} Hilbert bundle and a \textit{trivial} Hilbert bundle. The latter is a bundle which is literally a Cartesian product:

\[ \mathcal{H} = X \times \mathcal{H}_0 \]

(2.2)

with \( \pi \) the projection onto the first factor and \( \mathcal{H}_0 \) is a fixed separable Hilbert space, say \( \mathbb{C}^N \) for the finite-dimensional case and \( \ell^2(\mathbb{Z}) \) for the infinite-dimensional case. By contrast, a bundle \( \pi : \mathcal{H} \to X \) is \textit{trivializable} if there is a bundle isomorphism to the trivial bundle \( X \times \mathcal{H}_0 \). What this means, in practice, is that for all \( x \in X \) there is a basis \( \{\psi_{n,x}\} \) of the Hilbert space \( \mathcal{H}_x \) that varies “continuously” (or “smoothly” if we want to differentiate) as a function of \( x \). By choosing some basepoint \( x_0 \in X \) we can choose an isomorphism \( \mathcal{H}_{x_0} \cong \mathcal{H}_0 \) and then such a basis defines an isomorphism

\[ \Phi_{x_0,x} : \mathcal{H}_x \to \mathcal{H}_{x_0} \].

(2.3)

A trivializable bundle together with a choice of trivialization will be said to be \textit{trivialized}.

The distinction between trivializable and trivialized Hilbert bundles might seem like hopelessly arcane solipsistic mathematical hair-splitting to most physicists, but we will see that it can be important. A relevant preliminary remark is that if there are different trivializations of \( \mathcal{H} \) corresponding to choices of bases \( \{\psi_{n,x}\} \) and \( \{\tilde{\psi}_{n,x}\} \) then \( \Phi_{x_0,x} \circ \Phi_{x_0,x}^{-1} : X \to U(\mathcal{H}_0) \) can be a nontrivial map of \( X \) to the unitary group of \( \mathcal{H}_0 \). (It can even be topologically nontrivial, depending on the topology used to define the unitary group.)

2.2 Projected Bundles

Now suppose that \( P(x) : \mathcal{H}_x \to \mathcal{H}_x \) is a continuous family of projection operators. We can then define a sub-bundle \( \mathcal{V} \subset \mathcal{H} \) to be the vector bundle whose fiber above \( x \) is just the image of \( P(x) \) within \( \mathcal{H}_x \). Then \( \mathcal{V} \) is called the \textit{projected bundle} associated to the family of projection operators.

There is another useful way to think about projected bundles. Recall that a \textit{section} of \( \pi : \mathcal{H} \to X \) is a continuous map \( \Psi : X \to \mathcal{H} \) so that \( \pi(\Psi(x)) = x \). That is, a section is a continuous assignment of vectors

\[ x \mapsto \psi(x) \in \mathcal{H}_x \]

(2.4)

(We will generally denote sections by capital Greek letters like \( \Psi \) and the values of sections at \( x \) by lowercase Greek letters like \( \psi(x) \).) Now, we can define a projected bundle by saying what its space of sections is. The linear span of these sections at any \( x \) then defines the
fiber $V_x \subset H_x$. By definition, the space of sections $\Gamma(V)$ is the set of sections which are eigenvectors of $P(x)$ of eigenvalue 1 for all $x$:

$$\Gamma(V) := \{ \Psi \in \Gamma(H) : P(x)\psi(x) = \psi(x) \quad \forall x \}.$$  \hfill (2.5)

An important theorem, the Serre-Swan theorem, says that every finite dimensional vector bundle is isomorphic to a projected subbundle of some finite rank trivial Hilbert bundle.

### 2.3 Projected Connections

Let us first recall the definition of a connection on a vector bundle. A connection is simply a first-order differential operator on sections of $V$. That is, one can define a connection $\nabla$ on $V$ to be a map

$$\nabla : \Gamma(V) \rightarrow \Omega^1(V),$$  \hfill (2.6)

where $\Omega^1(V)$ is the space of one-forms on $X$ valued in $V$, such that the Leibniz rule is satisfied:

$$\nabla(f \Psi) = df \otimes \Psi + f \nabla(\Psi).$$  \hfill (2.7)

Here $f$ is an arbitrary differentiable function on $X$. Note that the difference of two connections is a one-form, valued in endomorphisms of the fibers of $V$. Indeed, the space of connections on a vector bundle $V$ is an affine space modeled on the vector space $\Omega^1(\text{End}(V))$. It has no natural choice of origin and hence there is no canonical connection on $V$. There is one important exception to this statement: If the vector bundle $V$ is trivial, $V = X \times V_0$ for some fixed vector space $V_0$ then there is a natural choice of origin, namely the trivial connection. To define it, choose any basis $v_n$ of $V_0$ so the general section is $\Psi = s^n v_n$ where $s^n$ is a tuple of functions on $X$. Then the trivial connection is defined by

$$\nabla^{\text{trivial}} \Psi = dx^\mu \frac{\partial s_n}{\partial x^\mu} \otimes v_n.$$  \hfill (2.8)

Now suppose that $V$ is presented as a projected subbundle of a Hilbert bundle $\pi : H \rightarrow X$, and we have chosen a connection $\nabla^H$ on $H$. Then we can define the projected connection:

$$\nabla^P := P \circ \nabla^H \circ \iota,$$  \hfill (2.9)

where $\iota : \Gamma(V) \rightarrow \Gamma(H)$ is the inclusion and $P : \Gamma(H) \rightarrow \Gamma(V)$ is the projection.

While the above definition of a connection is most convenient for defining projected connections, there is a more conceptual definition which will prove useful in section below. In this second definition a connection on a vector bundle $\pi : \mathcal{V} \rightarrow X$ is simply a rule for coherently lifting paths in $X$ to paths in $\mathcal{V}$. A “lifting” of a path $\gamma : [0, 1] \rightarrow X$ to a path $\tilde{\gamma} : [0, 1] \rightarrow \mathcal{V}$ is a path $\tilde{\gamma}$ such that $\pi(\tilde{\gamma}(t)) = \gamma(t)$. By “coherently lifting” we mean that the lifted paths satisfy natural composition laws. \footnote{To be a little more precise, a connection is a rule which takes a pair of data given by: (1.) a continuous path $\gamma : [0, 1] \rightarrow X$ connecting, say, $x_0$ to $x_1$ and (2.) a choice of initial vector $v_0 \in \pi^{-1}(x_0) = \mathcal{V}_{x_0}$ and returns a lifted path $\tilde{\gamma} : [0, 1] \rightarrow \mathcal{V}$ with $\tilde{\gamma}(0) = v_0$. The lifted path is required to satisfy a natural composition law.} The relation between the two definitions is

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this: To define a lifted path $\tilde{\gamma}(t)$ one solves the first order differential equation $\nabla_{\dot{\gamma}} \Psi = 0$, where $\dot{\gamma}$ is the tangent vector to $\gamma(t)$, using the initial condition $\tilde{\gamma}(0) = v_0$. It must be stressed that the projection of the lifted path in $\mathcal{H}$ from $\nabla^\mathcal{H}$ is in general not the lifted path in $\mathcal{V}$ from $\nabla^\mathcal{V}$! Indeed, even in the case that $\mathcal{H}$ is the trivial bundle and we use the trivial connection $\nabla^\mathcal{H} = \nabla^\text{trivial}$ the lifted path in $\mathcal{H}$ is $\tilde{\gamma}(t) = (\gamma(t), v_0)$ where $v_0$ is the initial vector in the fiber over $\mathcal{H}_{\gamma(0)}$. However the projected path $(\gamma(t), P(\gamma(t))v_0)$ will not be covariantly constant with respect to $\nabla^\mathcal{V}$ precisely because, in general, $PdP \neq 0$. In this way the projected connection can be nontrivial, even if $\nabla^\mathcal{H}$ is trivial.

A simple and popular example of a projected connection is given by choosing the Hilbert bundle

$$\mathcal{H} = S^2 \times \mathbb{C}^2$$

(2.10)

where we think of $S^2$ as the set of unit vectors in $\mathbb{R}^3$ and we choose the family of projection operators

$$P(\hat{x}) = \frac{1}{2}(1 + \hat{x} \cdot \vec{\sigma}).$$

(2.11)

In this case, if we take the trivial connection on $\mathcal{H}$ then the projected connection is just the magnetic monopole connection on a complex line bundle of first Chern class one.

We are finally ready to define Berry connections. Suppose then we have a Hilbert bundle $\pi : \mathcal{H} \to X$ and moreover we are given a continuously varying family of Hamiltonians $H_x$ acting on $\mathcal{H}_x$ so that there is an energy $E_{\text{gap}}$ that is not in the joint spectrum of all the Hamiltonians:

$$E_{\text{gap}} \notin \bigcup_{x \in X} \text{Spec}(H_x).$$

(2.12)

In this case we can define projection operators $P(x)$ to project onto the eigenstates of $H_x$ of energies below $E_{\text{gap}}$:

$$P(x) = \Theta(E_{\text{gap}} - H_x)$$

(2.13)

where $\Theta$ is the Heaviside step function. If we choose a connection $\nabla^\mathcal{H}$ on $\mathcal{H}$ then the projected connection is known, in physics, as a Berry connection:

$$\nabla^{\text{Berry}} := P \circ \nabla^\mathcal{H} \circ \iota.$$ 

(2.14)

The central point we are attempting to make in this note is simply to stress that the definition of the Berry connection depends on a choice of connection $\nabla^\mathcal{H}$ on $\mathcal{H}$. In general the Hilbert bundle $\mathcal{H}$ is trivializable, but there is no natural trivialization. When this is the case there is no natural origin in the affine space of connections on $\mathcal{H}$. In the original papers by M. Berry [2][3] and by B. Simon [34] it was assumed that $\mathcal{H}$ is the trivial bundle. In this case, as we have noted, there is a natural origin, namely the trivial connection on the composition rule so that composition of paths in the base corresponds to suitable composition of lifted paths. In equations, if $\gamma_{0,1}$ is a path from $x_0$ to $x_1$ and $\gamma_{1,2}$ is a path from $x_1$ to $x_2$ and we define $\gamma_{0,2}$ to be the composed path $\gamma_{0,1} \circ \gamma_{1,2}$ (with time running twice as fast) then if the choice of initial vector $v_0 \in \mathcal{V}_{x_0}$ defines a lift with endpoint $v_1 = \tilde{\gamma}_{0,1}(1)$ and we use $v_1$ as the initial vector for lifting $\gamma_{1,2}$ then the composition $\tilde{\gamma}_{0,1} \circ \tilde{\gamma}_{1,2}$ is the lift of $\gamma_{0,2}$ with initial vector $v_0$. Finally, the lifting must be linear: If the initial points $v_0$ and $v_0'$ lead to lifted paths $\tilde{\gamma}$ and $\tilde{\gamma}'$ then the initial point $v''_0 = v_0 + v_0'$ leads to a lifted path with $\tilde{\gamma}''(t) = \tilde{\gamma}(t) + \tilde{\gamma}'(t)$. The addition here means vector addition in the fiber above $\gamma(t)$. 

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and that is the connection implicitly used in those papers (and all subsequent papers of which we are aware). Thus, when one encounters expressions like

\[ A^{\text{Berry}} = \langle \psi | \nabla_R | \psi \rangle, \tag{2.15} \]

a trivialization has been assumed. Of course, the expression (2.15) has been used without incident in a wide variety of applications in molecular, and optical physics \[5, 33\]. The reason is that in the models used in these applications the statement of the problem includes a natural trivialization. For example, in the Born-Oppenheimer approximation in molecular physics the definition of the Hilbert space of the electrons does not depend on the positions of the nuclei (although the Hamiltonian most certainly does). Therefore the original Hilbert bundle over the control parameter space is literally a trivial bundle.

3. The Adiabatic Theorem Revisited

The Berry connection has its origin in the quantum adiabatic theorem \[2, 34\]. In this case we study the Schrödinger equation

\[ i\hbar \frac{\partial \Psi}{\partial t} = H(X(t))\Psi \tag{3.1} \]

where the \( X(t) \) are time-dependent control parameters, varying slowly on the time-scales set by the energies of the Hamiltonians \( H(X(t)) =: H(t) \). How do our current considerations enter into the adiabatic theorem? Although universally written (so far as we know), equation (3.1) is actually not completely sensible from a mathematical viewpoint: If the \( X(t) \) are varying then \( \Psi(t) \) must be a section of a bundle of Hilbert spaces and in particular, for each different \( X(t) \) the vector \( \Psi(t) \in \mathcal{H}_{X(t)} \) is in a different fiber of the Hilbert bundle.

If the bundle has not been trivialized then it does not make sense to write a derivative \( \frac{\partial \Psi}{\partial t} \) without a choice of connection on the bundle! The correct Schrödinger equation must actually be written as:

\[ i\hbar \nabla^\mathcal{H} \Psi = H(X(t))\Psi \tag{3.2} \]

where \( \nabla^\mathcal{H} \) is a contraction of the connection \( \nabla^\mathcal{H} \) on \( \mathcal{H} \) with the tangent vector to the path in the space of control parameters.

Now recall that the essence of the adiabatic theorem for (3.1) is that the natural parallel transport defined by the time-evolution operator \( U(t_1, t_2) = \text{Pexp} \left\{ \frac{1}{\hbar} \int_{t_1}^{t_2} H(t') dt' \right\} \) does not commute with the spectral projections for the Hamiltonians \( H(t_1) \) and \( H(t_2) \). However, if the variation of \( H(t) \) is “small” then the time-evolution operator has a “small” commutator with the spectral projections: The amplitudes for transitions between eigenspaces for different eigenvalues will be small. The same general discussion can be applied to (3.2) and of course the connection \( \nabla^\mathcal{H} \) must likewise be such that the associated parallel transport operators have “small” commutators with the spectral projections of \( H(t) \). When this holds the quantum adiabatic theorem can be generalized, and after removing the “dynamical phase” (for example, the factor \( \exp \left\{ \frac{1}{\hbar} \int E_n(t') dt' \right\} \) associated with an isolated eigenvalue \( E_n(t) \)) the remaining “geometric phase” is just the parallel transport operator associated with the projected connection for \( \nabla^\mathcal{H} \).
4. Band Structure

A simple example of a Hilbert bundle with no natural trivialization is provided by the familiar setting of band structure. Let \( C \subset \mathbb{A}^n \) be a crystal in affine \( n\)-dimensional space with Euclidean metric. We assume that \( C \) is invariant under translation by a rank \( n \) lattice \( L \subset \mathbb{R}^n \). We can then define the Brillouin torus \( T^\vee \) to be the space of unitary irreducible representations of \( L \). This is generally presented as \( T^\vee = \mathcal{K}/L^\vee \) where \( L^\vee := \text{Hom}(L, \mathbb{Z}) \) is the integral dual of \( L \) and \( \mathcal{K} \) is the vector space of momentum vectors. \( \mathcal{K} \) is also known as “reciprocal space.”

Mathematically, it can be identified with the cotangent space of \( \mathbb{A}^n \) at any point. We denote points of the Brillouin torus by \( \bar{k} \) so that the corresponding unitary representation of \( L \) can be presented as

\[
\chi_{\bar{k}}(R) = e^{2\pi i k \cdot R} \tag{4.1}
\]

for all \( R \in L \), where \( k \) is any lift of \( \bar{k} \) to \( \mathcal{K} \).

We can define a Hilbert bundle \( \pi : \mathcal{H} \rightarrow T^\vee \) whose fiber \( \mathcal{H}_{\bar{k}} \) is the space of Bloch functions on \( \mathbb{A}^n \):

\[
\psi(x + R) = e^{2\pi i k \cdot R} \psi(x) \tag{4.2}
\]

that are suitably normalizable. (They are \( L^2 \)-normalizable over a fundamental domain for the action of \( L \) on \( \mathbb{A}^n \).) Put differently, \( \mathcal{H}_{\bar{k}} \) is the space of \( L^2 \)-sections of the Poincaré line bundle \( L_{\bar{k}} \) over the torus \( T := \mathbb{A}^n/L \).

Now, there is no natural trivialization of \( \mathcal{H} \) simply because the definition of the fibers \( \mathcal{H}_{\bar{k}} \) depends on \( \bar{k} \). In discussions of band structure we are given a Schrödinger operator on \( L^2(\mathbb{A}^n) \) invariant under translation by \( L \) and then, under some circumstances, the eigenfunctions \( \{\psi_n, \bar{k}\} \) of the Schrödinger operator define a natural trivialization. Roughly speaking, below any finite energy the bands should not cross and should define a trivializable finite rank vector bundle. (In particular all the Chern classes and \( K \)-theory invariants should be trivial.) In general, bands do cross, and Chern numbers are nonzero. In such cases, there is certainly no natural trivialization of the Hilbert bundle.

Suppose now that we have an insulator, so that the Fermi energy \( E_f \) of the many-body ground state is in a gap separating filled (valence) bands from the unfilled (conduction) bands. This is a classic example of the situation in which we would like to define the Berry connection associated with the Hamiltonians \( H_{\bar{k}} \) acting on the Bloch functions with Bloch momentum \( \bar{k} \). In this case we have a natural projected bundle, \( \mathcal{F} \), the bundle of filled bands, defined by using \( P(\bar{k}) = \Theta(E_f - H_{\bar{k}}) \). However, as we just stressed, the Hilbert bundle has no natural trivialization, therefore, it would seem that there is no natural choice for \( \nabla^\mathcal{H} \) and hence there is no natural choice of the Berry connection. The situation is not quite that dire because, as noted in [15], there is in fact a natural family of connections \( \nabla^{\mathcal{H}, \bar{x}_0} \) whose gauge equivalence class is parametrized by the real-space torus: \( \bar{x}_0 \in \mathbb{A}^n/L \).

\(^3\)Here we differ from traditional solid state physics conventions where the inner product between a lattice and reciprocal lattice vector is \( 2\pi \) times an integer. In our conventions the inner product is integral. Consequently, there is an extra \( 2\pi \) in the formula for the Bloch phases below relative to what is standard in the condensed matter literature.
These connections have the distinguishing property that they are flat (zero curvature) and their holonomy only depends on the data at hand. They also show up in first order response theory.

We recall here the definition of $\nabla^{H,x_0}$ from [15]. Since the connections are all flat connections it suffices to define the parallel transport on straight-line paths and these can in turn be taken to be projections of paths in $\mathcal{K}$ given by

$$k(t) = k_0 + t \delta k \quad 0 \leq t \leq 1. \quad (4.3)$$

Let $\bar{\gamma}(t) = \overline{k(t)}$ denote the projection of the path (4.3) in $\mathcal{K}$ to a path in $T^\vee$. We need to define a lift of $\bar{\gamma}(t)$ to a path $\tilde{\gamma}(t)$ in $\mathcal{H}$, given an initial vector $\psi_{k_0} \in \mathcal{H}_{k_0}$. If we choose $x_0 \in \mathbb{A}^n$ then we can define $\tilde{\gamma}(t) = U^{\mathcal{H},x_0}(t)\psi_{k_0}$ to be the function on $\mathbb{A}^n$ whose value at $x$ is

$$(U^{\mathcal{H},x_0}(t) \cdot \psi_{k_0})(x) := e^{2\pi i \delta k \cdot (x-x_0)} \psi_{k_0}(x). \quad (4.4)$$

It is easily checked that $U^{\mathcal{H},x_0}(t)\psi_{k_0}$ has quasi-periodicity given by $\overline{k(t)}$ and that paths suitably compose. By computing the holonomy around small closed triangles one also easily checks that this is a flat connection. Note especially that since the crystal is in affine space we must subtract points $x - x_0$ in order to define a vector which can be paired with a reciprocal vector $\delta k \in \mathcal{K}$. It would not make sense to write this formula without $x_0$. If you do that, you are implicitly making an unphysical choice of origin. Thus, we need to choose a point $x_0$ in order to define the connection. The isomorphism class (= gauge equivalence class) of a flat connection is completely characterized by its holonomy. Using $\pi_1(T^\vee, \bar{k}_0) \cong L^\vee$ for each homotopy class we can choose the minimal length representative to be the projection of

$$k(t) = k_0 + tG \quad 0 \leq t \leq 1 \quad (4.5)$$

where $G \in L^\vee$ is a reciprocal lattice vector. Denote the corresponding closed curve in $T^\vee$ by $\gamma_G$. (The notation suppresses the dependence on the basepoint $\bar{k}_0$.) The holonomy around $\gamma_G$ is the multiplication of Bloch functions:

$$H^{x_0}(\gamma_G) : \psi_{k_0}(x) \mapsto e^{2\pi i G \cdot (x-x_0)} \psi_{k_0}(x). \quad (4.6)$$

The difference of holonomy operators for two choices of $x_0$ is

$$H^{x_0}(\gamma_G)(H^{x'_0}(\gamma_G))^{-1} = e^{-2\pi i G \cdot (x_0-x'_0)} 1_{\mathcal{H}_{k_0}} \quad (4.7)$$

and is proportional to the unit operator on $\mathcal{H}_{k_0}$. Note that $H^{x_0}(\gamma_G)$ only depends on the projection of $x_0$ to $T$. Thus the isomorphism classes of the connections $\nabla^{\mathcal{H},x_0}$ are parametrized by the real-space torus $T$.

Another way to say this is that if we view the connection $\nabla^{\mathcal{H},x_0}$ as a first order differential operator on $\Gamma(\mathcal{H})$ then the difference of two connections in the family is:

$$\nabla^{\mathcal{H},x_0} - \nabla^{\mathcal{H},x'_0} = 2\pi i dk \cdot (x_0-x'_0) \otimes 1_{\mathcal{H}}. \quad (4.8)$$

A shift of $x_0$ by a lattice vector $R \in L$ can be undone by a gauge transformation defined by conjugating all Bloch functions in $\mathcal{H}_{\bar{k}}$ by the unitary operator $U(\bar{k}) = e^{2\pi i k \cdot R}$. Thus,
we see again that the gauge equivalence class of $\nabla^{H,x_0}$ only depends on the projection of $x_0$ to $\bar{x}_0 \in T$. If we now consider an insulator with a bundle of filled bands $\mathcal{F}$ then the projected connections associated to a Fermi energy $E_f$ together with a choice $\nabla^{H,x_0}$ on $\mathcal{H}$ gives us a corresponding family of Berry connections $\nabla^{\mathcal{F},x_0}$ such that
\[
\nabla^{\mathcal{F},x_0} - \nabla^{\mathcal{F},x_0'} = 2\pi i d k \cdot (x_0 - x_0') \otimes 1_{\mathcal{F}}.
\] (4.9)
Again, the gauge equivalence classes of these connections are parametrized by the real space torus $T$. If one thinks of the Berry connection in band theory as just given by the expectation value of the position operator then the dependence on a choice of origin is completely obvious.

The subtlety we are stressing here can often, but not always, be ignored. It is important to distinguish a crystal $C \subset \mathbb{A}^n$ in an affine space with no distinguished origin from a lattice $L \subset \mathbb{R}^n$, which does have a distinguished origin. If $L$ acts transitively on $C$ (that is, there is just one atom per unit cell) then there is a natural choice for $\bar{x}_0$, provided by the equivalence class of the points $C$ itself. In this case there is a distinguished Berry connection. Moreover, the difference of the connections in (4.9) is a flat one-form proportional to the unit operator on the fibers of $\mathcal{F}$. Thus the difference might seem a bit trivial, and indeed the field strengths $F(\nabla^{\mathcal{F},x_0})$ are independent of $x_0$. Therefore the Chern-Weil representatives of Chern classes are independent of $x_0$. (This is in harmony with the fact that the Chern classes of $\mathcal{F}$ cannot depend on any choice of connection on $\mathcal{F}$.) Nevertheless, in general, the gauge equivalence class of a connection on a vector bundle is not completely captured by the fieldstrength. Two classic examples of gauge invariant information not captured by the fieldstrength are holonomy around nonbounding closed cycles and Chern-Simons invariants. Both of these examples show up in the physics of insulators. We will now discuss these two examples.

5. Example 1: Electric Polarization

There is a famous formula for the contribution of the valence electrons in an insulator to the zero-temperature electric polarization per unit volume, $P$. It must be admitted that, in fact, $P$ is not quite well-defined. Only differences of $P$ are really well-defined. Nevertheless there is a useful expression for $P$, defined up to shifts by $\frac{e}{\Omega} L$, where $\Omega$ is the volume of a unit cell of $L$, from which one can derive the physically relevant differences of $P$ resulting from a change in control parameters. The “momentum space” expression (equation (8b) of [20] or equation (19) of [32]) can be written in the form:
\[
G \cdot P = \frac{e}{2\pi i} \int_{T^\vee, \perp} \log \det \text{Hol}(\nabla^{\mathcal{F},x_0}(\gamma_G)) \, \mathrm{d} \text{vol} \mod \frac{e}{\Omega} \mathbb{Z}
\] (5.1)
where $G$ is an arbitrary reciprocal lattice vector and $\gamma_G$ is the corresponding closed loop in $T^\vee$. We have written this in terms of the holonomy of the Berry connection, $\text{Hol}(\nabla^{\mathcal{F},x_0}(\gamma_G))$ to emphasize the gauge invariance of the result. $T^\vee, \perp$ is the subtorus through the origin.

\footnote{In general $\gamma_G$ depends on a choice of basepoint $\bar{k}_0$, and if we choose $\bar{k}_0 \neq 0$ we should choose the subtorus through that point. More on that below.}
and orthogonal to \( G \) and it carries a natural volume form \( d\text{vol} \) inherited from the Euclidean metric on \( A^3 \). The expression (5.1) involves taking a logarithm of the gauge-invariant holonomy of the Berry connection, and consequently \( P \) is only defined modulo \( \frac{e}{\Omega} \) times a lattice vector. The ambiguity of \( P \) under shifts in \( \frac{e}{\Omega}L \) is well-appreciated and widely discussed in the literature, and the physical origin of this ambiguity is well-understood. See, for example [20, 32, 31]. On the other hand, the expression also depends continuously on \( x_0 \) since:

\[
P(x_0) - P(x'_0) = \frac{e}{\Omega} (x_0 - x'_0).
\]

This is completely distinct from the usual ambiguity of the polarization by \( \frac{e}{\Omega}L \) discussed in the literature. On the other hand, the ambiguity (5.2), is also physically rather trivial: It is exactly what we expect for the dependence of electric polarization on a choice of origin if we only take into account the contribution of the electrons - all of which have the same sign! The physically relevant result must take into account the contribution of the neutralizing positive charges of the ions as in equation (20) of [32].

**Remarks**

1. The derivation of (5.1) begins with a Kubo formula for the variation of polarization as a function of control parameters in some space \( X \) [30]. The Kubo formula was used to define a one-form \( dP \) on the product \( T^\vee \times X \). It was observed in [28] that this one-form in fact has nonzero periods, and a relation to Berry’s phase was noted. In [20] it was observed that a local anti-derivative of the one-form can be written in a form equivalent to (5.1), and it is in this step, where one passes from Berry curvature to holonomy, that the \( x_0 \) dependence enters.

2. In some cases when one has a global trivialization \( \{\psi_{n,\bar{k}}\} \) of \( \mathcal{H} \) one can introduce a set of “Wannier functions”:

\[
W_{n,R} := \frac{1}{(2\pi)^3} \int_{T^\vee} \chi^*_k(R) \psi_{n,\bar{k}} \ d\text{vol}
\]

(5.3)

In such cases there is an alternative “real space” expression (see equation (10) of [20]). These real-space expressions make the dependence of \( P \) on a choice of origin obvious, and we have now explained where that dependence resides in the reciprocal space version of the formula, namely equation (5.1). (We also note in passing that (5.3) only makes sense when we can choose a global trivialization, and then only because \( \psi_{n,\bar{k}} \) can be viewed as a quasiperiodic function on \( A^n \) and it makes sense to add such functions. In general it does not make mathematical sense to add vectors in different fibers of a bundle. Rather, one must use a connection to parallel transport these vectors to a common fiber, where they can be added. Thus, in general, one might attempt to choose a basepoint \( \bar{k}_0 \in T^\vee \), and a flat connection, such as \( \nabla^\mathcal{H},x_0 \) and a choice of paths \( \gamma_{\bar{k},\bar{k}_0} \) from \( \bar{k} \in T^\vee \) to \( \bar{k}_0 \) and write

\[
W_{n,R} := \frac{1}{(2\pi)^3} \int_{T^\vee} \chi^*_k(R) U^\mathcal{H},x_0(\gamma_{\bar{k},\bar{k}_0}) \psi_{n,\bar{k}} \ d\text{vol}
\]

(5.4)
A natural way to choose paths is to choose a fundamental domain for \( L^\vee \) in \( K \) and use straight-line paths from \( \bar{k}_0 \) to the boundaries. Nevertheless, this is not totally satisfactory since the result will still depend on the choice of fundamental domain.

3. In the case of a Chern insulator, where the Berry curvature has periods, the expression \( (5.1) \) has further dependence on the basepoint of the closed loop \( \gamma^C \). Thus it is necessary to specify further data to obtain a meaningful expression for \( P^{[10]} \).

6. Example 2: Axion Angle

As a second example we consider the case of the magneto-electric polarizability response tensor for an insulator in 3 + 1 dimensions. This can be defined as the leading term in the low energy effective action for the Maxwell gauge field in the presence of an insulator:

\[
S_{\text{eff}} \sim \frac{1}{\hbar} \int_{\mathbb{R}^4} \alpha^{ij} E_i B_j + \cdots \tag{6.1}
\]

where \( E_i \) and \( B_j \) are the components of the electric and magnetic fields of an external Maxwell gauge field probing the insulator. In a rather beautiful development \([13, 14, 35]\), it was noted that the trace part of \( \alpha^{ij} \) (to be thought of as an “axion angle”) is related to the Chern-Simons invariant of “the” Berry connection on the Brillouin torus. Since there is, in general, no distinguished Berry connection we must choose one, and the ones which arise from first order response theory come from the family of connections \( \nabla^{F,x_0} \) described above. So we write the theta angle in terms of the Chern-Simons invariant of this connection:

\[
\theta(x_0) = \frac{1}{3} \alpha^{ii} = \int_{T^\vee} \text{CS}(\nabla^{F,x_0}). \tag{6.2}
\]

Our normalization of the Chern-Simons invariant is that \( \theta \) is defined modulo 2\( \pi \). In \([13, 14, 35]\) the \( x_0 \) dependence was not included. In the case of insulators with time-reversal invariance or parity invariance the connection must be compatible with the lift of \( P \) or \( T \) to \( F \) and, as is well-known, the Chern-Simons invariant is either 0 or \( \pi \) modulo 2\( \pi \). Indeed, one can define a strong topological insulator as a parity or time-reversal invariant insulator with \( \theta = \pi \). However, for a general insulator there is no natural choice of basepoint \( x_0 \).

Quite generally, under a shift of connection \( \nabla \to \nabla + \alpha \), where \( \alpha \) is a one-form valued in endomorphisms of the vector bundle, the Chern-Simons form changes by

\[
\text{CS}(\nabla + \alpha) - \text{CS}(\nabla) = \text{Tr} \left( 2\alpha F + \alpha \nabla \alpha + \frac{2}{3} \alpha^3 \right). \tag{6.3}
\]

We use this equation with \( \alpha = 2\pi i dk \cdot (x'_0 - x_0) 1_F \) as in \((4.9)\) to obtain

\[
\text{CS}(\nabla^{F,x_0'}) = \text{CS}(\nabla^{F,x_0}) + 4\pi i dk \cdot (x'_0 - x_0) \wedge \text{Tr} F(\nabla^{F,x_0}). \tag{6.4}
\]

In our conventions, \( \text{Tr} F(\nabla^{F,x_0}) \) is \( \frac{1}{2} \) times the Chern-Weil representative of the first Chern class \( c_1(F) \) of \( F \). The first Chern class \( c_1(F) \) can be integrated over a basis of homology.
two-cycles in $T^\lor$ to produce a three-component vector. In fact this vector can be understood more invariantly by interpreting the expression

$$\int_{T^\lor} c_1(\mathcal{F})$$

as a vector in the reciprocal lattice $L^\lor$ as follows: Recall that $H_1(T^\lor; \mathbb{Z}) \cong L^\lor$. Therefore $H^1(T^\lor; \mathbb{Z}) \cong L$ and hence $H^2(T^\lor; \mathbb{Z}) \cong L \wedge L$. Therefore we can interpret the map $H^1(T^\lor; \mathbb{Z}) \to \mathbb{Z}$ defined by

$$\omega \mapsto \int_{T^\lor} \omega \wedge c_1(\mathcal{F}) \in \mathbb{Z}$$

as:

$$L \wedge c_1(\mathcal{F}) \to L \wedge L \cong \mathbb{Z}$$

where in the second step we paired with the fundamental class of $T^\lor$. (Of course, one can also evaluate the integral directly using local expressions to arrive at the same result.) We will denote the resulting reciprocal lattice vector by $G_{CH}$ and refer to it as the Chern-Halperin vector. The net result is that the dependence of the axion angle on origin is simply:

$$\theta(x_0) - \theta(x_0') = 2\pi G_{CH} \cdot (x_0 - x_0') \text{mod} 2\pi.$$

How should we interpret the dependence on $x_0$? One natural way is to interpret the statement as saying that for a three-dimensional Chern insulator the axion angle must be linear in space with proportionality constant given by the Chern-Halperin vector. The axion angle is periodic, so in this effective theory a remnant of the lattice periodicity remains in the periodicity under shifts of $x$ by a lattice vector. With this interpretation we can integrate by parts so that the axion angle term in the effective action for the Maxwell gauge field leads to a factor in the path integral:

$$\exp \left[ \frac{i}{4\pi} \left( \frac{e}{\hbar c} \right)^2 \int_{\mathbb{R}^4} (G_{CH} \cdot dx) \wedge A \wedge dA \right]$$

where we have expressed the result in cgs (Gaussian) units and $A$ is the gauge potential for the Maxwell fieldstrength. Differentiating with respect to $A_i$ gives the contribution to the current:

$$J^i = \frac{e^2}{\hbar} \epsilon^{ijk} (G_{CH})_j E_k$$

where again we stress that we are using cgs units and $(G_{CH})_j$ is a reciprocal vector to the lattice vectors so that $G_{CH} \cdot R \in \mathbb{Z}$ for all $R \in L$. This is the three-dimensional quantum Hall effect of [18, 21].

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5I thank Edward Witten for an essential discussion about this point.
6.1 A Pseudo-Topological Field Theory

The dimensionless action for the electromagnetic field (in cgs units) is

\[
S = \frac{1}{\hbar c} \int \frac{1}{8\pi} F \wedge \ast F - \left( \frac{e}{\hbar c} \right)^2 \int \frac{G_{CH} \cdot dx}{4\pi} \wedge A \wedge F
= \frac{1}{8\pi \hbar c} \int (F \wedge \ast F - G \wedge A \wedge F)
\]  

(6.11)

where we have defined a closed one-form on spacetime \( G \) given by

\[
G := \frac{2e^2}{\hbar c} G_{CH} \cdot dx
\]

in the rest-frame of the crystal. By power counting of momenta the action (6.9) should give the leading long-distance physics. However, the action

\[
\int G \wedge A \wedge dA
\]

(6.12)

is singular, even after allowing for gauge invariance: There is a zero mode under \( A \rightarrow A + \lambda G \), where \( \lambda \) is any real number. The situation is a little reminiscent of Costello’s discussion of integrable lattice models [11]. In order to have a nonsingular theory we must include the Maxwell action and hence the 3 + 1 dimensional theory is only “partially topological.” In momentum space the action is

\[
S = \frac{1}{8\pi \hbar c} \int \frac{d^4k}{(2\pi)^4} A^\mu (-k) D_{\mu\nu} A^\nu(k)
\]

(6.13)

with

\[
D_{\mu\nu} = (\eta_{\mu\nu} k^2 - k_\mu k_\nu) + i\epsilon_{\mu\nu\lambda\rho} G^\lambda k^\rho
\]

(6.14)

We can only hope to invert \( D_{\mu\nu} \) on a space orthogonal to the gauge modes, so we look for \( P^{\nu\lambda} \) such that

\[
D_{\mu\nu} P^{\nu\lambda} = \delta_\mu^\lambda - \frac{k_\mu k_\lambda}{k^2}.
\]

(6.15)

Now \( P^{\nu\lambda} \) must be a linear combination of the tensors:

\[
P^{\nu\lambda} = F_1 \eta^{\nu\lambda} + F_2 k^{\nu} k^{\lambda} + F_3 k^{\nu} G^{\lambda} + F_4 G^{\nu} k^{\lambda} + F_5 G^{\nu} G^{\lambda} + F_6 \epsilon^{\nu\lambda\omega\sigma} G_\varsigma k_\omega
\]

(6.16)

where \( F_1, \ldots, F_6 \) are functions of \( k^2, G^2, (G \cdot k) \). Imposing the condition (6.13) the functions \( F_2 \) and \( F_3 \) are undetermined while the remaining functions are uniquely determined. The function \( F_3 \) is determined by requiring \( P^{\nu\lambda}(k) \) to be symmetric under \( \nu \leftrightarrow \lambda \) and \( k \rightarrow -k \) and the choice of \( F_2 \) is a choice of gauge. Putting \( F_2 = 0 \) we get:

\[
-i P^{\nu\lambda} = \frac{k^2 \eta^{\nu\lambda} - \frac{G_{\nu\lambda}}{k^2} (G^{\nu} k^{\lambda} + k^{\nu} G^{\lambda}) + G^{\nu} G^{\lambda} - i\epsilon^{\nu\lambda\omega\sigma} G_\varsigma k_\omega}{G^2 k^2 - (G \cdot k)^2 + k^4}
\]

(6.17)

In Euclidean signature the denominator does not vanish, by the Cauchy-Schwarz inequality.

---

\(^6\)We are adding the Maxwell action in free space. It would make more sense to include a general permeability tensor in the first term to take into account the electromagnetic response of the material. However, to keep things simple we will ignore this point.
If we count derivatives in the action (6.11) then we might naively expect the Chern-Simons term to dominate in the infrared ($k \to 0$) limit. This is not quite true since the numerator of the propagator has terms of order zero in the $k$-expansion. But if we consider polarizations orthogonal to $G$ then indeed as $k \to 0$ we find a propagator scaling like $1/k^2$, similar to the standard propagator in Chern-Simons perturbation theory:

$$P^{\nu\lambda} \sim \frac{\epsilon^{\nu\lambda\omega} G_\zeta k_\omega}{G^2 k^2 - (G \cdot k)^2} \quad (6.18)$$

so long as we restrict attention to momenta $k$ not parallel to $G$. Note the singularity when $k \parallel G$. Like Hamlet, who is but mad north-north-west, the $k \to 0$ limit of the theory is only non-topological in the direction (in momentum space) parallel to $G$.

### 6.2 Dislocations

It was already noted in [18] that in the presence of dislocations of the three-dimensional crystal there will be interesting “edge modes” localized at those dislocations. A particularly obvious case is that of a screw dislocation along an axis (say, the $z$-axis) of a stack of two-dimensional Chern insulators. In this case, if we cut a small hole out around the dislocation with a helical boundary then the familiar edge modes will be localized on that helix. A general approach to the theory of such modes can be found in [1]. A related result for helical modes in topological insulators can be found in [19, 27]. Here we discuss the subject using the derivation of edge modes explained, for example, in [12, 24, 25, 36]. It just implements the anomaly inflow mechanism of Callan and Harvey [7]. The Chern-Simons term is anomalous under singular gauge transformations of electromagnetism, singular on the dislocation line. The anomaly must be cancelled by modes on a “cosmic string” or, in more modern language, on a “surface defect” in the effective gauge theory.\(^7\)

In the normal plane to a dislocation line the lattice has a locally-defined infinitesimal displacement by a vector $u(\phi)$ (where $\phi$ is an angular coordinate in the normal bundle) such that

$$\oint d\phi \frac{du}{d\phi} := D \in L \quad (6.19)$$

where $D$ is known as a Burgers vector. Thanks to (6.8) the axion angle has the property that

$$\oint d\theta = 2\pi G_{CH} \cdot D. \quad (6.20)$$

Now, a singular gauge transformation for the $U(1)$ electromagnetic field $g(\phi) = e^{i\phi}$ leads to an anomalous change in the action by

$$(G_{CH} \cdot D) \int_\Sigma F \quad (6.21)$$

on the worldsurface $\Sigma$ of the surface defect. This can be canceled by $G_{CH} \cdot D$ chiral modes located on the surface defect, thus confirming the general arguments of [3, 18].

\(^7\)This terminology could potentially be confusing: What high energy physicists call “surface defects” would be called “line defects” in condensed matter theory. We will deprecate the term “line defects” (in the condensed matter sense) in favor of “dislocation lines.”
6.3 Speculation: A 3+1-Dimensional FQHE

The 3+1 dimensional QHE is often dismissed as “uninteresting” because there is a natural layer structure given by the planes in the crystal orthogonal to $G$ and, it is claimed, it is “just” a stack of 2d Chern insulators, and there will be no phase transition as interlayer couplings are increased. However, having expressed the effective theory of the 3+1 QHE in the form (6.11) there is an obvious generalization, given the well-known formulation of the 2+1 dimensional FQHE in terms of abelian spin Chern-Simons theory [1, 4, 16, 17, 29, 37].

We choose a symmetric matrix of one-forms $K_{IJ}$ where each matrix element is defined by reciprocal lattice vectors and introduce an abelian gauge theory for a torus, with gauge fields $a^I$ (relative to a basis for the Lie algebra of the torus) and finally we choose a vector of one-forms defined by reciprocal lattice vectors $Q_I$ and consider the action:

$$\int K_{IJ} \wedge a^I \wedge da^J + Q_I \wedge da^I \wedge A \quad (6.22)$$

It would be amusing to explore the physical implications of such a phase of matter, and whether it can be realized by interacting electrons in 3+1 dimensions. In general, if the $K_{IJ}$ do not all point in the same direction there is no reason why this should behave like a stack of FQHE systems.

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