Geometry of gerbes and topological insulators

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II. BUNDLE GERBES WITH CONNECTION AND THEIR HOLONOMY

- Bundle gerbes with (unitary) connection are 1-degree higher structures as compared to line bundles with connection.
- They were introduced by Michael K. Murray in J. London Math. Soc. (2) 54 (1996), 403-416, as simple geometric examples of more abstract gerbes of J. Giraud (1971) and J.-L. Brylinski (1993).
- They were applied in physics to describe topological Wess-Zumino amplitudes in conformal field theory and string theory.
- Here I shall discuss how they relate to the topological insulators studied in condensed matter physics.

Definition. A bundle *gerbe* $\mathcal{G}$ with unitary connection (below, *gerbe* for short) over manifold M is a quadruple $(Y, B, \mathcal{L}, t)$ s.t.
- Y is a manifold equipped with a surjective submersion $\pi : Y \to M$
- B is a 2-form on Y
- $\mathcal{L}$ is a line bundle with hermitian structure and unitary connection over $Y^{[2]} \equiv Y \times_M Y$ with curvature $p_2^*B - p_1^*B$ where $p_{1,2}$ are the two projections from $Y^{[2]}$ to Y
- t is a smooth bilinear groupoid multiplication on $\mathcal{L}\rightrightarrows Y$

$$\mathcal{L}_{y_1,y_2} \times \mathcal{L}_{y_2,y_3} \xrightarrow{\ t\ } \mathcal{L}_{y_1,y_3}$$

where $\mathcal{L}_{y_1,y_2}$ denotes the fiber of $\mathcal{L}$ over $(y_1, y_2) \in Y^{[2]}$.

- Necessarily, $dB = \pi^*H$ where H is a closed 3-form on M called the *curvature* of the gerbe $\mathcal{G}$.
- Gerbes over M form a 2-category with 1-morphisms $\eta : \mathcal{G}_1 \longrightarrow \mathcal{G}_2$ and 2-morphisms $\mu : \eta_1 \longrightarrow \eta_2$ between a pair of 1-morphisms $\eta : \mathcal{G}_1 \longrightarrow \mathcal{G}_2$. 1-isomorphic gerbes have the same curvature.
- As line bundles, gerbes may be tensored (with curvatures adding up) or pulled back.
- The set of 1-isomorphism classes of flat gerbes (i.e. with zero curvature) over M is naturally isomorphic to $H^2(M, U(1))$.
- A gerbe $\mathcal{G}$ with curvature 3-form H exists iff H has periods in $2\pi\mathbb{Z}$.
- In the latter case, there is a free transitive action of $H^2(M, U(1))$ on the set of 1-isomorphism classes of gerbes over M with fixed curvature form H generated by the tensor product with flat gerbes.
- If Σ is an oriented closed 2-surface and $\phi : \Sigma \longrightarrow M$ is a smooth then for any gerbe $\mathcal{G}$ over M,

$$\phi^*\mathcal{G} \in H^2(\Sigma, U(1)) \cong U(1).$$

The corresponding phase in $U(1)$ is called the holonomy of $\mathcal{G}$ along the map ϕ and is denoted $Hol_{\mathcal{G}}(\phi)$. Physicists' name for $Hol_{\mathcal{G}}(\phi)$ is the Wess-Zumino amplitude of ϕ.

- If there exists an extension of ϕ to a map $\widetilde{\phi}:\widetilde{\Sigma}\longrightarrow M$ from an oriented 3-manifold $\widetilde{\Sigma}$ with the boundary $\partial\widetilde{\Sigma}=\Sigma$ then

$$Hol_{\mathcal{G}}(\phi)\ =\ \exp\Big[\mathrm{i}\int\limits_{\widetilde{\Sigma}}\widetilde{\phi}^*H\Big].$$

III. SQUARE ROOT OF THE GERBE HOLONOMY

Suppose that $\mathcal{G}$ is a gerbe over M with curvature H and $\Theta:M\longrightarrow M$ is an involution.

Definition. A Θ-equivariant structure on $\mathcal{G}$ is composed of
- a 1-isomorphism $\eta:\mathcal{G}\longrightarrow\Theta^*\mathcal{G}$
- a 2-isomorphism $\mu:\Theta^*\eta\circ\eta\longrightarrow Id_{\mathcal{G}}$ between 1-isomorphisms of gerbe $\mathcal{G}$ s.t.
- there is an equality $Id_\eta\circ\mu=\Theta^*\mu\circ Id_\eta$ of the 2-isomorphisms between the 1-isomorphisms $\eta\circ\Theta^*\eta\circ\eta:\mathcal{G}\longrightarrow\Theta^*\mathcal{G}$ and $\eta:\mathcal{G}\longrightarrow\Theta^*\mathcal{G}$.

- Note that the existence of a Θ-equivariant structure on $\mathcal{G}$ implies that $\Theta^*H=H$.
- Let $\vartheta:\Sigma\longrightarrow\Sigma$ be an *orientation-preserving* map with a non-empty discrete set of fixed points. **Examples:** for the 2-torus $\mathbb{R}^2/(2\pi\mathbb{Z}^2)\equiv\mathbb{T}^2$ one may take ϑ generated by $k\mapsto -k$ for $k\in\mathbb{R}$; for the hyperelliptic curve given by the equation $y^2=p(z)$ one may take $\vartheta(y,z)=(-y,z)$.
- We shall call a smooth map $\phi:\Sigma\longrightarrow M$ equivariant if $\phi\circ\vartheta=\Theta\circ\phi$.

Proposition. If the fixed point set $M'\subset M$ of Θ is connected and simply connected then a Θ-equivariant structure on a gerbe $\mathcal{G}$ over M permits to fix an unambiguous square root $\sqrt{Hol_{\mathcal{G}}(\phi)}$ of the holonomy of $\mathcal{G}$ along equivariant maps $\phi:\Sigma\longrightarrow M$.

- If there exists an extension $\widetilde{\phi}:\widetilde{\Sigma}\longrightarrow M$ of ϕ and an *orientation-preserving* involution $\widetilde{\vartheta}:\widetilde{\Sigma}\longrightarrow\widetilde{\Sigma}$ reducing to ϑ on $\partial\widetilde{\Sigma}=\Sigma$ s. t. $\widetilde{\phi}\circ\widetilde{\vartheta}=\Theta\circ\widetilde{\phi}$ then

$$\sqrt{Hol_{\mathcal{G}}(\phi)}\ =\ \exp\Big[\tfrac{\mathrm{i}}{2}\int\limits_{\widetilde{\Sigma}}\widetilde{\phi}^*H\Big].$$

- We shall call a gerbe $\mathcal{G}$ over M equipped with a Θ-equivariant structure a Θ-equivariant gerbe.

IV. A $3d$ INDEX

- Let R be an oriented compact 3-manifold without boundary and $\rho:R\longrightarrow R$ an *orientation-reversing* involution with a non-empty set of fixed points. **Example:** for the 3-torus $\mathbb{R}^3/(2\pi\mathbb{Z}^3)\equiv\mathbb{T}^3$ we may take ρ generated by $k\mapsto -k$ for $k\in\mathbb{R}^3$.
- We shall call a smooth map $\Phi:R\longmapsto M$ equivariant if $\Phi\circ\rho=\Theta\circ\Phi$.
- Let $F\subset R$ be the closure of a fundamental domain for ρ that is a submanifold with boundary of R. Then ρ preserves ∂F together with its orientation inherited from R.
  Example: for $R=\mathbb{T}^3$ with ρ generated by $k\mapsto -k$ we may take $F=[0,\pi]\times\mathbb{T}^2$ with ∂F composed of two connected components: $\{\pi\}\times\mathbb{R}^2/(2\pi\mathbb{Z}^2)$ and $\{0\}\times\mathbb{R}^2/(2\pi\mathbb{Z}^2)$.

Proposition. Let $\mathcal{G}$ be a Θ-equivariant gerbe over M with curvature H and $\Phi:R\longrightarrow M$ an equivariant map. If the fixed-point set $M'\subset M$ is connected and simply connected then the ratio

$$\frac{\exp\Big[\frac{\mathrm{i}}{2}\int\limits_F\Phi^*H\Big]}{\sqrt{Hol_{\mathcal{G}}(\Phi|_{\partial F})}}\ \equiv\ \mathcal{K}_{\mathcal{G}}(\Phi)$$

taking the values ±1 is independent of the choice of the fundamental domain $F\subset R$.

V. BASIC GERBE OVER $U(N)$

- For the condensed matter applications, we shall need to apply the above general constructions to the case where $M = U(N)$ and $H = \frac{1}{12\pi}\,\mathrm{tr}(V^{-1}dV)^3$ is the closed bi-invariant 3-form on $U(N)$ normalized so that its set of periods is $2\pi\mathbb{Z}$.
- A gerbe $\mathcal{G}$ on $U(N)$ with curvature H is called *basic*. It is unique up to 1-isomorphisms.
- We use a construction of such a gerbe adapted from from a 2008 paper of Murray-Stevenson based on the ambiguities in taking the logarithm of a unitary matrix.
- In this construction, $\mathcal{G} = (Y, B, \mathcal{L}, t)$ where
  - $Y = \big\{(\epsilon, V) \in]-2\pi, 0[\times U(N) \mid \mathrm{e}^{-\mathrm{i}\epsilon} \notin spec(V)\big\}$ with $\pi : Y \longrightarrow U(N)$ forgetting ϵ
  - B such that $dB = \pi^* H$ is defined from the Poincaré Lemma using the homotopy $h : [0,1]\times Y \longrightarrow Y$

$$h(t, \epsilon, V) = (\epsilon, \mathrm{e}^{-\mathrm{i}tH_\epsilon(V)})$$

    where $H_\epsilon(V) = \mathrm{i}\ln_{-\epsilon} V$ with the cut in $\ln_{-\epsilon}$ at the argument $-\epsilon$
  - For $\epsilon_1 \leq \epsilon_2$,

$$H_{\epsilon_1}(V) - H_{\epsilon_2}(V) = 2\pi P_{\epsilon_1,\epsilon_2}(V)$$

    where $P_{\epsilon_1,\epsilon_2}(V)$ is the spectral projector of V on the subspace $E_{\epsilon_1,\epsilon_2}(V) \subset \mathbb{C}^N$ corresponding to the eigenvalues $\mathrm{e}^{-\mathrm{i}e}$ with $\epsilon_1 < e < \epsilon_2$. One takes

$$\mathcal{L}_{\epsilon_1,\epsilon_2,V} \;=\; \wedge^{max} E_{\epsilon_1,\epsilon_2}(V)$$

    for the fiber of line bundle $\mathcal{L}$ over $(\epsilon_1, \epsilon_2, V) \in Y^{[2]}$
  - The connection on $\mathcal{L}$ is essentially the Berry one (slightly modified)
  - The groupoid multiplication t on $\mathcal{L} \rightrightarrows Y$ is induced by the isomorphism

$$\wedge^{max} E_{\epsilon_1,\epsilon_2}(V) \;\otimes\; \wedge^{max} E_{\epsilon_2,\epsilon_3}(V) \;\cong\; \wedge^{max} E_{\epsilon_1,\epsilon_3}(V)$$

    for $\epsilon_1 \leq \epsilon_2 \leq \epsilon_3$.

VI. TIME-REVERSAL ON $U(N)$

- In quantum mechanics with the space of states $\mathbb{C}^N$, the time reversal is realized by an anti-unitary map $\theta : \mathbb{C}^N \longrightarrow \mathbb{C}$ such that $\theta^2 = \pm I$.
- For the plus sign, one can take for θ the complex conjugation whereas for the minus sign, θ exists only for N even and can be taken as the product of the unitary Pauli matrices σ_2 placed diagonally and the complex conjugation.
- In both cases, θ induces an involution $\Theta : U(N) \longrightarrow U(N)$ by the formula $\Theta(V) = \theta V \theta^{-1}$ and $\Theta^* H = H$ for the bi-invariant 3-form H considered above.

Proposition. 1. If $\theta^2 = I$ then the basic gerbe $\mathcal{G}$ over $U(N)$ may be equipped with the Θ-equivariant structure. However, in this case the the set of fixed points under Θ is isomorphic to $O(N)$ and is neither connected nor simply connected.
2. If $\theta^2 = -I$ then there is no Θ-equivariant structure on the basic gerbe $\mathcal{G}$ over $U(N)$. However Θ lifts to the involution $\widehat{\Theta}$ on the double cover $\widehat{U}(N)$ of $U(N)$ and there exists a $\widehat{\Theta}$-equivariant structure on the pullback $\widehat{\mathcal{G}}$ to $\widehat{U}(N)$ of the basic gerbe over $U(N)$. The fixed-point set of $\widehat{\Theta}$ is isomorphic to two disjoint copies of $Sp(N)$ and is simply connected.

- For $\theta^2 = I$ the lack of 1-connectivity of the fixed point set does not allow to define the square root $\sqrt{Hol_{\mathcal{G}}(\phi)}$ nor of the $3d$ index $\mathcal{K}(\Phi)$ for equivariant maps ϕ and Φ.
- For $\theta^2 = -I$, every equivariant map $\phi : \mathbb{T}^2 :\longrightarrow U(N)$ and every equivariant map $\Phi : \mathbb{T}^3 \longrightarrow U(N)$ may be lifted to an equivariant map $\widehat{\phi} : \mathbb{T}^2 :\longrightarrow \widehat{U}(N)$ and $\widehat{\Phi} : \mathbb{T}^3 :\longrightarrow \widehat{U}(N)$ and one can still define uniquely $\sqrt{Hol_{\widehat{\mathcal{G}}}(\widehat{\phi})}$ and $\mathcal{K}(\widehat{\phi})$ in spite of the lack of connectivity of the fixed point set of $\widehat{\Theta}$. Besides these quantities do not depend on the choice of the lifts $\widehat{\phi}$ and $\widehat{\Phi}$. We shall then use the notation $\sqrt{Hol_{\mathcal{G}}(\phi)}$ and $\mathcal{K}(\Phi)$ for them.

Remark. The last point, however, does not hold for arbitrary $(\Sigma.\vartheta)$ and (R, ρ).

VII. APPLICATION TO TOPOLOGICAL INSULATORS

- In the simplest case, the d-dimensional insulators are described by lattice Hamiltonians that, after the discrete Fourier(-Bloch) transformation, give rise to a map
$$\mathbb{T}^d \ni k \;\longmapsto\; H(k) = H(k+G) \;\in\; End(\mathbb{C}^N)$$
with $G \in 2\pi\mathbb{Z}^d$ and all the Hermitian matrices $H(k)$ have a spectral gap around the Fermi energy ϵ_F. We shall denote by $P(k) = P(k+G)$ the spectral projectors on the eigenstates of $H(k)$ with energies $< \epsilon_F$.
- For the time-reversal symmetric insulators,
$$\theta H(k)\theta^{-1} = H(-k) \qquad \text{and} \qquad \theta P(k)\theta^{-1} = P(-k)$$
where $\theta^2 = -I$.
- We shall denote by $V_P(k)$ the unitary matrix $I - 2P(k)$. Note that in two or three dimensions, the map $\mathbb{T}^d \ni k \;\longmapsto\; V_P(k) \in U(N)$ is then equivariant, i.e. $\Theta(V_P(k)) = V_P(-k)$.

Theorem. 1. For $d = 2$, $\sqrt{Hol_{\mathcal{G}}(V_P)} = (-1)^{KM}$ where $KM \in \mathbb{Z}_2$ is the Kane-Mele (2005) invariant of the time-reversal symmetric $2d$ topological insulators.
2. For $d = 3$, $\mathcal{K}(V_P) = (-1)^{KM^s}$ where $KM^s \in \mathbb{Z}_2$ is the *strong* Fu-Kane-Mele (2007) invariant of the time-reversal symmetric $3d$ topological insulators.

- The physical importance of the Kane-Mele invariants relies on the fact that they count the parity of the number of massless modes carrying topological protected currents localized near the boundary that appear once we put the lattice system in a half-infinite space. This is the bulk-edge correspondence.

VIII. APPLICATION TO FLOQUET SYSTEMS

- Floquet systems are described by lattice Hamiltonians periodically depending on time that after the discrete Fourier(-Bloch) transformation, give rise to a map
$$\mathbb{R} \times \mathbb{T}^d \ni (t,k) \;\longmapsto\; H(t,k) = H(t+1,k) = H(t,k+G) \;\in\; End(\mathbb{C}^N)$$
where we fixed the period of temporal driving to 1.
- The evolution of such systems is described by the unitary matrices $U(t,k)$ such that
$$\mathrm{i}\partial_t U(t,k) = H(t,k)\,U(t,k), \qquad U(0,k) = I, \qquad U(t+1,k) = U(t,k)U(1,k).$$
- Suppose that $\epsilon \in [-2\pi, 0[$ is such that $\mathrm{e}^{-\mathrm{i}\epsilon} \notin spec(U(1,k))$ for all k. Then $H_\epsilon(U(1,k)) = \mathrm{i}\ln_{-\epsilon}(U(1,k))$ is well defined and
$$V_\epsilon(t,k) = U(t,k)\,\mathrm{e}^{-\mathrm{i}tH_\epsilon(U(1,k))} = V_\epsilon(t+1,k)$$
may be viewed as a periodized evolution.
- For $\epsilon_1 \leq \epsilon_2$,
$$H_{\epsilon_2}(U(1,k)) - H_{\epsilon_1}(U(1,k)) = 2\pi P_{\epsilon_1,\epsilon_2}(U(1,k)).$$
- For the time-reversal symmetric Floquet systems
$$\theta H(t,k)\theta^{-1} = H(-t,-k), \qquad \theta U(t,k)\theta^{-1} = \Theta(U(t,k)) = U(-t,-k)$$
where $\theta^2 = -I$.
- It follows that
$$\theta H_\epsilon(U(1,k))\theta^{-1} = H_\epsilon(U(1,-k)), \qquad \Theta(V_\epsilon(t,k)) = V_\epsilon(1-t,-k).$$
and for $\epsilon_1 \leq \epsilon_2$,
$$\theta P_{\epsilon_1,\epsilon_2}(U(1,k))\theta^{-1} = P_{\epsilon_1,\epsilon_2}(U(1,-k)).$$
- In particular, in $2d$ one may consider the Kane-Mele invariants $KM_{\epsilon_1,\epsilon_2} \in \mathbb{Z}_2$ given by the relation

$$(-1)^{KM_{\epsilon_1,\epsilon_2}} = \sqrt{Hol_{\mathcal{G}}(V_{P_{\epsilon_1,\epsilon_2}})}$$

where $V_{P_{\epsilon_1,\epsilon_2}}(k) = I - 2P_{\epsilon_1,\epsilon_2}(U(1,k))$ depend only on the time-1 evolution operators $U(1,k)$.

Definition. In $2d$ take $R = \mathbb{R}/\mathbb{Z} \times \mathbb{T}^2$ with the *orientation-reversing* involution $\rho(t,k) = (1-t,-k)$. Then $V_\epsilon : R \longrightarrow U(N)$ is an equivariant map and we define the additional dynamical topological invariants $K_\epsilon \in \mathbb{Z}_2$ of the gapped time-reversal symmetric Floquet system by the relation

$$(-1)^{K_\epsilon} = \mathcal{K}(V_\epsilon).$$

Proposition. The above invariants are related by the identity

$$K_{\epsilon_2} - K_{\epsilon_1} = KM_{\epsilon_1,\epsilon_2}.$$

- Similarly in $3d$ we may define the *strong* Fu-Kane-Mele invariants $KM^s_{\epsilon_1,\epsilon_2} \in \mathbb{Z}_2$ depending on $U(1,k)$ by

$$(-1)^{KM^s_{\epsilon_1,\epsilon_2}} = \mathcal{K}(V_{P_{\epsilon_1,\epsilon_2}}).$$

Definition. In $3d$ take $R = \mathbb{T}^3$ with the *orientation-reversing* involution $\rho(k) = (-k)$. Then $V_\epsilon|_{t=\frac{1}{2}} : R \longrightarrow U(N)$ is an equivariant map and we define the additional dynamical topological invariants $K^s_\epsilon \in \mathbb{Z}_2$ of the time-reversal symmetric gapped Floquet system by the relation

$$(-1)^{K^s_\epsilon} = \mathcal{K}(V_\epsilon|_{t=\frac{1}{2}}).$$

Proposition. The $3d$ invariants are related by the identity

$$K^s_{\epsilon_2} - K^s_{\epsilon_1} = KM^s_{\epsilon_1,\epsilon_2}.$$

- The indices K_ϵ and K^s_ϵ seem to count the parity of the number of current-carrying eigen-modes of the time-1 evolution operator that are localized near the boundary of the half-space lattice system that appear in the bulk spectral gap around $\mathrm{e}^{-\mathrm{i}\epsilon}$.

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