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MATHEMATICAL PROBLEMS IN THE THEORY OF TOPOLOGICAL INSULATORS

ROSTOV - 2022

I. INTRODUCTION

Our talk is devoted to one of the most interesting and actively developing themes in the condensed matter physics — the theory of topological insulators. We have chosen this particular topic since, apart from its importance in theoretical physics, we were attracted by the numerous connections of this theory with various directions in modern mathematics including topology and homotopy theory, Clifford algebras and K-theory, non-commutative geometry and C^*-algebras.

The role of topology in the theory of condensed matter first became clear in the study of the quantum Hall effect starting from the papers by Loughlin and Thouless et al. The topological insulators are characterized by the wide energy gap, stable under small deformations, which motivates the application of topological methods.

A key point in the study of topological objects in the solid state physics is played by their symmetry groups. There are three basic types of symmetries, namely the time reversion symmetry, preservation of the number of particles (or charge symmetry) and PH-symmetry (particle-hole symmetry). The description of the symmetries arising in solid state physics goes back to Kitaev who proposed the classification of topological insulators based on this study.

In our talk we pay main attention to the topological insulators invariant under time reversion.

II. BLOCH THEORY

Classical Bloch theory describes the properties of solid bodies having the crystal lattice called Bravais lattice. From mathematical point of view it is a discrete Abelian group Γ in the space $\mathbb{R}^d$ with $d = 3$ isomorphic to $\mathbb{Z}^d$ and acting on $\mathbb{R}^d$ by translations T_γ generated by vectors $\gamma \in \Gamma$.

The behavior of free electrons in a solid body is determined by the one-particle Schrödinger equation

$$H\psi := (-\Delta + V)\psi = E\psi$$

with periodic potential V invariant under the action of Γ. Such operator commutes with all operators T_γ.

Denote by Γ' the dual lattice in the momentum space $(\mathbb{R}^d)'$ defined in the following way:

$$\Gamma' = \{k \in (\mathbb{R}^d)' : k \cdot \gamma \in 2\pi \mathbf{Z} \quad \text{for all } \gamma \in \Gamma\}.$$

The fundamental domain (unit cell) $M_{\Gamma'}$ of the lattice Γ' is called the Brillouin zone Br_d.

The functions, invariant under Γ, may be considered as functions on the torus $\mathbb{T}^d = \mathbb{R}^d/\Gamma$. Denote by $\mathcal{H}_0$ the Hilbert space

$$\mathcal{H}_0 = L^2(\mathbb{T}^d) = L^2(\mathbb{R}^d/\Gamma)$$

with respect to the measure on $\mathbb{R}^d/\Gamma$ induced by the Lebesgue measure dx on $\mathbb{R}^d$. The exponential $e_k = e^{ik\cdot x}$ belongs to $\mathcal{H}_0$ if $k \in \Gamma'$. Moreover, such functions form an orthonormal basis in $\mathcal{H}_0$.

The smooth functions of the form

$$\psi(x) = e^{ik\cdot x}\varphi(x),\ x \in \mathbb{R}^d,$$

where the vector k belongs to the Brillouin zone Br_d and the function $\varphi \in C^\infty(\mathbb{R}^d/\Gamma)$, are called the Bloch functions and the vector k is called the quasimomentum. The space of Bloch functions with quasimomentum k is denoted by L_k.

The Schrödinger operator acts on Bloch functions by the formula

$$H\left(e^{ik\cdot x}\varphi(x)\right) = e^{ik\cdot x}H_k\varphi(x).$$

The operator H_k, called the effective or Bloch Hamiltonian, has the form

$$H_k\varphi = (\frac{1}{i}\nabla + k)^2\varphi + V\varphi.$$

The operator H_k maps the space $C^\infty(\mathbb{R}^d/\Gamma)$ to itself. It implies that the original Schrödinger operator $H = H_0$ maps the space of Bloch functions with quasimomentum k to itself.

If we denote by I_k the operator of multiplication by $e^{ik\cdot x}$ then the above formula may be rewritten in the form

$$I_k^{-1} H I_k = H_k.$$

In other words,

$$H|_{L_k} = I_k \circ H_k|_{L_0} \circ I_k^{-1}.$$

In this way the study of the operator $H|_{L_k}$ is reduced to the study of the operator $H_k|_{L_0}$.

Denote by $H(k)$ the closure of the operator $H_k|_{L_0}$ in the space $\mathcal{H}_0$. The definition domain of this operator coincides with the subspace

$$D(H(k)) = \{\varphi : \varphi(x) = \sum_{\gamma' \in \Gamma'} c_{\gamma'} e^{i(\gamma', x)} \text{ such that } \sum_{\gamma' \in \Gamma'} (1 + |\gamma'|^2)|c_{\gamma'}|^2 < \infty\}.$$

This subspace may be identified with the Sobolev space $H^2(\mathbb{R}^d/\Gamma)$ provided with the inner product

$$\|\varphi\|_2^2 = V_\Gamma \sum_{\gamma' \in \Gamma'} (1 + |\gamma'|^2)^2 |\varphi_{\gamma'}|^2$$

where V_Γ is the volume of the fundamental domain M_Γ of the lattice Γ.

The spectrum of operator $H(k)$ is discrete and its eigenfunctions $\varphi_m(k)$, being solutions of the equation

$$H(k)\varphi_m(k) = E_m(k)\varphi_m(k),$$

form a complete orthogonal system in the Hilbert space $\mathcal{H}_0$.

The collection of energy levels, corresponding to the eigenvalues $E_m(k)$ with fixed m, is called the energy zone. So the eigenfunctions $E_m(k)$ determine the zonal structure of the solid body.

The ground state of the system with n levels has the following structure. There is a number p of completely occupied one-electron levels with energy not exceeding the quantity E_F, called the Fermi energy. Above it there are $n - p$ empty (non-occupied) levels. The interval between the highest occupied level and the lowest empty level is called the energy gap or forbidden zone. The solid bodies with wide energy gap, stable under small deformations, are called the insulators.

The Bloch functions

$$\psi_{m,k}(x) = e^{ik\cdot x}\varphi_{m,k}(x),$$

are the eigenfunctions of the original Schrödinger operator H.

Denote by $\mathcal{H}_k$ the completion of the space L_k with respect to the norm determined by the isomorphism $I_k : L_0 \to L_k$ so that I_k extends to the isometry $I_k : \mathcal{H}_0 \to \mathcal{H}_k$. Consider the vector bundle $\pi : \mathfrak{H} \to \mathrm{Br}_d$ with the fibre $\mathcal{H}_k$ over the point $k \in \mathrm{Br}_d$ and denote by $\mathcal{H} = L^2(\mathfrak{H})$ the Hilbert space of square integrable sections of $\mathfrak{H}$ with inner product

$$(s_1, s_2) = \int_{\mathrm{Br}_d} (s_1(k), s_2(k))dk$$

where $(s_1(k), s_2(k))$ is the inner product in $\mathcal{H}_k$. The space $\mathcal{H}$ is the direct integral of Hilbert spaces $\mathcal{H}_k$ over the space Br_d with measure dk.

III. TOPOLOGICAL INVARIANTS

Let $H(k)$ be the Bloch Hamiltonian describing the zonal insulator with forbidden zone on the level of Fermi energy E_F. We can diagonalize it by unitary conjugation:

$$U^*(k)H(k)U(k) = \mathrm{diag}(E_1(k), \ldots, E_n(k)).$$

Suppose that the first m levels $E_i(k) > E_F$, $i = 1, \ldots, m$, are empty and the occupied levels correspond to the energies $E_i(k) < E_F$ with $i = m + 1, \ldots, n$ where $n \gg 1$.

There exists the adiabatic deformation of this Hamiltonian, i.e. its continuous deformation in the class of considered Hamiltonians not affecting the forbidden zone, to a Hamiltonian with only two energy values equal for all occupied (resp. free) levels to -1 (resp. +1). (This deformation may be given by an explicit formula using the spectral decomposition.)

In other words, there exists a matrix $U(k)$ such that

$$U^*(k)H(k)U(k) = \mathrm{diag}\left(1_{m\times m}, -1_{(n-m)\times(n-m)}\right).$$

Note that the matrix $U(k)$ in this equation is defined only up to transformations of the form

$$U(k) \longmapsto U(k)\mathrm{diag}\left(U_{m\times m}, U_{(n-m)\times(n-m)}\right).$$

Hence, the matrix $U(k)$, yielding a solution of the above equation, determines a map from the Brillouin zone $\mathrm{Br}_d = \mathbb{T}^d$ to the Grassmannian

$$\mathrm{Gr}_{m,n} = \mathrm{U}(n)/\mathrm{U}(m) \times \mathrm{U}(n-m).$$

So we have arrived at the problem of description of homotopy classes $[\mathbb{T}^d, \mathrm{Gr}_{m,n}]$ of maps from the torus $\mathbb{T}^d$ to Grassmann manifolds.

The general problem of description of the homotopy equivalence classes $[\mathbb{T}^d, X]$ of continuous maps from $\mathbb{T}^d$ to topological spaces X was studied by Fox.

The structure of the space $[\mathbb{T}^d, X]$ is determined by the collection of the maps

$$\Omega_I^r : \pi_r(X) \to [\mathbb{T}^d, X]$$

with $r \le d$. These maps are parameterized by the ordered subsets $I = \{i_1 < \ldots < i_r\}$ in the set of indices $\{1, \ldots, d\}$. Accordingly, the elements of $[\mathbb{T}^d, X]$ are parameterized by the collections of d elements from the group $\pi_1(X)$, $\frac{d(d-1)}{2}$ elements from $\pi_2(X), \ldots,$ $\binom{d}{j}$ elements from $\pi_j(X)$ and so on.

Return to the above problem of the description of homotopy classes $[\mathbb{T}^d, \mathrm{Gr}_{m,n}]$ of the maps of the torus $\mathbb{T}^d$ to Grassmann manifolds.

Applying the Fox construction to the Grassmannian $\mathrm{Gr}_{m,n}$, we get for $d = 1$: $[\mathbb{T}^1, \mathrm{Gr}_{m,n}] = \pi_1(\mathrm{Gr}_{m,n}) = 0$, for $d = 2$ the homotopy classes of the maps $\mathbb{T}^2 \to \mathrm{Gr}_{m,n}$ are characterized by the unique invariant since $\pi_2(\mathrm{Gr}_{m,n}) = \mathbb{Z}$, and for $d = 3$ the homotopy classes of the maps $\mathbb{T}^3 \to \mathrm{Gr}_{m,n}$ are classified by three elements from the group $\pi_2(\mathrm{Gr}_{m,n}) = \mathbb{Z}$ since $\pi_1(\mathrm{Gr}_{m,n}) = \pi_3(\mathrm{Gr}_{m,n}) = 0$.

Non-trivial classes in dimensions $d = 2, 3$ are described in the following way. The space $[\mathbb{T}^d, \mathrm{Gr}_{m,n}]$ may be considered as the classifying space for the bundles over $\mathbb{T}^d$. In dimension $d = 2$ there is a non-trivial bundle over $\mathbb{T}^2$ analogous to the Hopf bundle over $\mathbb{S}^2$. From the physical point of view this case corresponds to the quantum spin Hall state. In dimension $d = 3$ there are three bundles over $\mathbb{T}^3$ which are the pullbacks of the Hopf bundle with respect to three different projections $\mathbb{T}^3 = \mathbb{S}^1 \times \mathbb{S}^1 \times \mathbb{S}^1 \mapsto \mathbb{T}^2 = \mathbb{S}^1 \times \mathbb{S}^1$.

IV. T-SYMMETRY

Consider now the time reversion symmetry in more detail. This symmetry is given by the T-transform, i.e. by the operator T which satisfies the condition $T^2 = -\mathrm{id}$ and is anti-unitary in the sense that

$$(T\varphi, T\psi) = (\psi, \varphi)$$

for any states φ, ψ. It implies, in particular, that the state φ and its T-partner $T\varphi$ are orthogonal to each other: $(\varphi, T\varphi) = 0$.

Indeed,

$$(T\varphi, \varphi) = -(T\varphi, T^2\varphi) = -(T\varphi, \varphi)$$

where the last equality follows from the anti-unitarity of T.

Since these states have the same energy it means that any energy eigenstate is double degenerated. This effect is called the Kramers degeneration.

V. INVOLUTIVE SPACES

The topological insulators with the time reversal symmetry are described mathematically in terms of involutive spaces. From this moment our exposition becomes more abstract and accordingly we change some notations. In particular, the momentum space of a topological insulator is denoted further on by X with its points denoted by x. We also suppose that X is a connected compact topological space. For example, if the coordinate space is determined by the lattice in $\mathbb{R}^d$, as in the first part of this talk, then its momentum space is the torus $\mathbb{T}^d$.

Definition

The involutive space (X, τ) is a topological space X provided with the involution, i.e. a homeomorphism $\tau : X \to X$ with the square $\tau^2 = \mathrm{id}_X$.

Such space is also called the R-space. Here is an example of the R-space

$$\mathbb{R}^{p,q} := \mathbb{R}^q + i\mathbb{R}^p$$

with coordinates $y + ix = (y, x)$. The involution on this space is given by the map $\tau : (y, x) \mapsto (y, -x)$.

The T-symmetry in the involutive space X is usually given by the change of signs of local coordinates. For example, if the sphere $\mathbb{S}^d$ is realized as the unit sphere in the space $\mathbb{R}^{d+1}$ with coordinates $(x_0, x_1, \ldots, x_d)$, satisfying the relation $x_0^2 + x_1^2 + \ldots + x_d^2 = 1$, then it is natural to define the T-symmetry on it by the map $(x_0, x_1, \ldots, x_d) \mapsto (x_0, -x_1, \ldots, -x_d)$. For the torus $\mathbb{T}^d = \mathbb{S}^1 \times \ldots \times \mathbb{S}^1$ with coordinates $(e^{i\theta_1}, \ldots, e^{i\theta_d})$ the T-symmetry is given by the map: $(e^{i\theta_1}, \ldots, e^{i\theta_d}) \mapsto (e^{-i\theta_1}, \ldots, e^{-i\theta_d})$.

The set of fixed points of involution τ on X is the set

$$X^\tau = \{x \in X : \tau(x) = x\}.$$

We suppose that it consists of a finite number of points. In the above example of the sphere $\mathbb{S}^d$ the involution τ has two fixed points $(\pm 1, 0, \ldots, 0)$ while the involution on torus $\mathbb{T}^d$ has 2^d fixed points given by the collections $(\varepsilon_1, \ldots, \varepsilon_d)$ of $\varepsilon_i = \pm 1$.

VI. HILBERT BUNDLE OF TOPOLOGICAL INSULATOR

Recall that we denote by $\pi : \mathfrak{H} \to X$ the Hilbert bundle of the topological insulator over the momentum space $X = \mathrm{Br}_d$. The fibre of this bundle at the point $x \in X$ is the Hilbert space $\mathcal{H}_x$ and we denote by $\mathcal{H} = L^2(\mathfrak{H})$ the Hilbert space of its square integrable sections. These sections are identified with the physical states with eigenfunctions $E(x)$.

The time reversion transform on the space $\mathcal{H}$ is given by the operator Θ which is an anti-unitary operator, satisfying the conditions: $\Theta^2 = -1$ and $\Theta^* = -\Theta$.

Definition

The Q-bundle (E, ρ) over the involutive space (X, τ) is a complex vector bundle $E \to X$ provided with the anti-involution ρ compatible with τ. The anti-involution ρ is given by the anti-linear bundle isomorphism $\rho : E \to E$ such that $\rho^2 = -\mathrm{id}_E$.

The compatibility condition of ρ and involution τ means that $\pi \circ \rho = \tau \circ \pi$. At fixed points $x \in X^\tau$ the map $\rho_x : E_x \to E_x$ is an anti-linear map with $\rho_x^2 = -\mathrm{id}_{E_x}$. So ρ_x defines a quaternionic structure (action of quaternions) on E_x.

If we replace in this definition the anti-involution ρ by the involution σ such that $\sigma^2 = \mathrm{id}_E$ then we obtain the definition of the R-bundle (E, σ) over (X, τ).

The Hilbert bundle $\pi : \mathfrak{H} \to X$, provided with the time reversion operator Θ, becomes the Q-bundle $\pi : (\mathfrak{H}, \Theta) \to (X, \tau)$. In other words, the involution τ is pulled up to the anti-involution Θ on the Hilbert bundle $\pi : \mathfrak{H} \to X$.

The Hamiltonian $H(x)$, invariant under time reversion, should satisfy the condition

$$\Theta H(x)\Theta^* = H(\tau(x)),\ x \in X.$$

Hence, If φ is an eigenstate of H, i.e. $H(x)\varphi(x) = E(x)\varphi(x)$, then $\Theta\varphi$ is an eigenstate of $\Theta H\Theta^*$ with the same energy E:

$$[\Theta H\Theta^*]\Theta\varphi(x) = E(\tau(x))\Theta\varphi(x).$$

In other words, the states φ and $\Theta\varphi$ belong to the same zone with energy E. So every zone under the T-symmetry is double degenerated and $(\varphi, \Theta\varphi)$ form the Kramers pair.

In this case the rank of the Hilbert bundle $\mathfrak{H}$ is even, i.e. equal to $2N$ where N is a natural number. If T is the only symmetry of $\mathfrak{H}$, i.e. every zone is precisely doubly degenerated, then $\mathfrak{H}$ is represented in the form

$$\mathfrak{H} = \bigoplus_{i=1}^{N} \mathfrak{H}_i$$

where $\mathfrak{H}_i$ are subbundles of $\mathfrak{H}$ of rank 2 with the spaces of sections $\Gamma(X, \mathfrak{H}_i)$ generated by the global Kramers sections $(\varphi_i, \Theta\varphi_i)$.

Denote by $w_i : X \to \mathrm{U}(2)$ the transition function of the bundle $\mathfrak{H}_i$. The T-transform on $\mathfrak{H}$ changes w_i to $w_i \circ C$ where C is the complex conjugation. In terms of local coordinates (x, v) on $\mathfrak{H}_i$ the operator Θ acts by the formula: $(x, v) \mapsto (\tau(x), w_i(x)\bar{v})$. Using the relation $\Theta^2 = -\mathrm{id}_{\mathfrak{H}_i}$, we arrive at the equality

$$w_i(\tau(x))\bar{w}_i(x) = -\mathrm{id}_{\mathcal{H}_i}, \text{ i.e. } w_i^t(\tau(x)) = -w_i(x).$$

In particular, at fixed points $x \in X^\tau$ the matrix $w_i(x)$ is skew-symmetric.

In the case when $X = \mathbb{S}^3 = \{(\alpha, \beta) \in \mathbb{C}^2 : |\alpha|^2 + |\beta|^2 = 1\}$ the T-symmetry is given by the formula: $\tau(\alpha, \beta) = (\bar{\alpha}, -\beta)$. Its fixed points are $(\pm 1, 0)$ and the transition function $w : \mathbb{S}^3 \to \mathrm{U}(2)$ is given by

$$w(\alpha, \beta) = \begin{pmatrix} \beta & \alpha \\ -\bar{\alpha} & \beta \end{pmatrix}$$

VII. MAJORANA ZERO MODES AND ANALYTICAL $\mathbb{Z}_2$-INDEX

Let $H(x)$ be a one-particle Hamiltonian on the momentum space X. It is T-invariant if

$$\Theta H(x)\Theta^* = H(\tau(x)),\ x \in X.$$

For topological insulators the Hamiltonian $H(x)$ at a fixed point $x_0 \in X^\tau$ may be approximated by the Dirac operator with a quadratic error term.

Consider the case when the Hilbert bundle $\pi : \mathfrak{H} \to X$ has rank 2 and its space of global sections is generated by the Kramers sections φ and $\Theta\varphi$. This pair of sections, having the same energy, may be considered as a quasiparticle composed of φ and $\Theta\varphi$. Its effective Hamiltonian has the form

$$\tilde{H}(x) = \begin{pmatrix} 0 & \Theta H(x)\Theta^* \\ H(x) & 0 \end{pmatrix} .$$

The Hamiltonian $\tilde{H}$ is T-invariant and the equation for the eigenvector φ of H with eigenvalue E takes in terms of $\tilde{H}$ the following matrix form

$$\begin{pmatrix} 0 & \Theta H(x)\Theta^* \\ H(x) & 0 \end{pmatrix} \begin{pmatrix} \varphi(x) \\ \Theta\varphi(x) \end{pmatrix} = \begin{pmatrix} E(\tau(x))\Theta\varphi(x) \\ E(x)\varphi(x) \end{pmatrix} .$$

Suppose that on the space of sections of the bundle $\mathfrak{H}$ it is given a real structure I satisfying the conditions: $I^2 = \mathrm{id}$, $I^* = I$.

Definition

A state ψ is called the Majorana state with respect to the real structure I if it satisfies the reality condition: $I\psi = \psi$.

Using the time reversion operator Θ, we can construct a real structure on $\mathcal{H}$ by setting

$$\mathcal{I} = \begin{pmatrix} 0 & \Theta^* \\ \Theta & 0 \end{pmatrix} .$$

It acts on the Kramers pair $\Phi = (\varphi, \Theta\varphi)$ by the formula

$$\begin{pmatrix} 0 & \Theta^* \\ \Theta & 0 \end{pmatrix} \begin{pmatrix} \varphi(x) \\ \Theta\varphi(x) \end{pmatrix} = \begin{pmatrix} \varphi(x) \\ \Theta\varphi(x) \end{pmatrix}$$

So $\Phi = (\varphi, \Theta\varphi)$ is the Maiorana state with respect to the real structure $\mathcal{I}$.

Definition

The Majorana zero mode is the Majorana state $\Phi_0 = (\varphi_0, \Theta\varphi_0)$, defined in a small neighborhood of a fixed point $x_0 \in X^\tau$, such that $\varphi(x_0) = \Theta\varphi(x_0) = 0$, changing the sign at this point.

Suppose that the operator H, hence also $\tilde{H}$, is Fredholm. The operator $H(x)$ near the fixed point x_0 is the sum of the Dirac operator and quadratic error term which does not affect the homotopy class. So the index of the topological insulator is determined by the index of Dirac operator at fixed points.

In a neighborhood of a fixed point x_0 the operator $\tilde{H}$ may be approximated by the Dirac operator which corresponds in the matrix form to the operator

$$\mathcal{D} = \begin{pmatrix} 0 & -D \\ D & 0 \end{pmatrix} .$$

So the operator $\tilde{H}$ near the fixed point x_0 is represented as the sum of the skew-symmetric operator $\mathcal{D}$ and quadratic error term which has no impact on the index of operator $\tilde{H}$ at this point.

For real skew-symmetric elliptic operators P Atiyah and Singer defined their analytical Z_2-index as

$$\mathrm{ind}_a P = \dim_{\mathbb{R}} \mathrm{Ker}\, P \bmod 2.$$

So it is natural to define the Z_2-invariant of a topological insulator as the sum

$$\nu = \sum_{x \in X^\tau} \mathrm{ind}_a \tilde{H}(x) = \sum_{x \in X^\tau} \dim\, \mathrm{Ker}\, \tilde{H}(x) \bmod 2$$

of local Z_2-indices at fixed points.

In physical terms the $\mathbb{Z}_2$-invariant ν is equal to the sum of the parities of the numbers of Majorana zero modes taken over all fixed points $x \in X^\tau$.

VIII. TOPOLOGICAL $\mathbb{Z}_2$-INDEX

Consider the construction of the topological $\mathbf{Z_2}$-index for the 3-dimensional involutive space (X, τ). Suppose that the Hilbert bundle $\pi : \mathfrak{H} \to X$ has rank 2 and the gauge group coincides with U(2). The anti-involution Θ on the Hilbert bundle $(\mathfrak{H}, \Theta) \to (X, \tau)$ is compatible with the natural involution ϑ on U(2) given by the formula: $\vartheta(g) = -g^t$, in the sense that $w \circ \tau = \vartheta \circ w$ where w is the transition function. In other words, w defines the equivariant map $w : (X, \tau) \to (\mathrm{U}(2), \vartheta)$.

The odd Chern character of a smooth map $g: X \to \mathrm{U}(n)$ is defined by the formula

$$\mathrm{Ch}(g) = \sum_{k=0}^{(d-1)/2} \mathrm{Ch}_{2k+1}(g) = $$
$$= \sum_{k=0}^{(d-1)/2} (-1)^k \frac{k!}{(2k+1)!} \mathrm{tr}\left[(g^{-1}dg)^{2k+1}\right].$$

Using this formula in the 3-dimensional case we can introduce the topological index

$$\mathrm{ind}_t g = \frac{1}{4\pi^2} \int_X \mathrm{Ch}_3(g) = \frac{1}{24\pi^2} \int_X \mathrm{tr}(g^{-1}dg)^3.$$

This number is also called the rotation number of the map g.

Due to T-symmetry the topological index $\mathrm{ind}_t w$ of the transition function w is defined modulo $\mathbb{Z}_2$.

The assertion that the topological $\mathbb{Z}_2$-index for 3-dimensional topological insulators coincides with the analytical $\mathbb{Z}_2$-index, i.e.

$$\nu = \mathrm{ind}_t w,$$

may be considered as an analog of Atiyah-Singer index theorem in our situation.

Another definition of topological $\mathbb{Z}_2$-index was proposed by Kane and Mele. This invariant, called the KM-invariant, is defined by the formula

$$\mathrm{KM}(X) = \prod_{x \in X^\tau} \frac{\mathrm{pf}[w(x)]}{\sqrt{\det[w(x)]}} \ .$$

As it was pointed out before, the transition function $w(x)$ at fixed points $x \in X^\tau$ is a skew-symmetric matrix so its pfaffian, denoted by $\mathrm{pf}[w(x)]$, is correctly defined. As we shall prove, the introduced KM-invariant coincides with the product of signs of pfaffians over all fixed points.

Recall the definition of pfaffian. Let $A = (a_{ij})$ be a skew-symmetric $(2n) \times (2n)$-matrix. Associate with it the bivector

$$\Omega = \sum_{i<j} a_{ij} e_i \wedge e_j$$

where $\{e_i\}$ is the standard orthonormal basis in $\mathbb{R}^{2n}$. Then the pfaffian $\mathrm{pf}(A)$ of the matrix A is defined by the equality

$$\frac{1}{n!}\Omega^n = \mathrm{pf}(A) e_1 \wedge \ldots \wedge e_{2n}.$$

The pfaffian $\mathrm{pf}(A)$ has the following properties:

1. $\mathrm{pf}(A)^2 = \det(A),\ \mathrm{pf}(\lambda A) = \lambda^n \mathrm{pf}(A);$
2. $\mathrm{pf}(BAB^t) = \det(B)\mathrm{pf}(A),\ \mathrm{pf}(A^t) = (-1)^n \mathrm{pf}(A).$

It is well known that the square matrix A satisfies the identity

$$\ln \det(A) = \operatorname{tr} \ln(A).$$

In the case when the matrix A is skew-symmetric this identity transforms into

$$2 \ln \operatorname{pf}(A) = \operatorname{tr} \ln(A).$$

The relation between the KM-invariant and the topological $\mathbb{Z}_2$-index is established using the following formula due to Kaufmann et al.

$$\sum_{x \in X^\tau} \ln \mathrm{pf}[w(x)] = \frac{1}{2}\, \mathrm{ind}_t w.$$

By exponentiating this equality we obtain the equation relating the product of pfaffians with the topological $\mathbb{Z}_2$-index

$$\prod_{x \in X^\tau} \mathrm{pf}[w(x)] = \exp\{2\pi i \frac{\mathrm{ind}_t w}{2}\} = (-1)^{\mathrm{ind}_t w}.$$

By setting the determinant $\det[w(x)]$ at fixed points $x \in X^\tau$ equal to 1, we get that $\mathrm{pf}[w(x)]$ at such points is equal to 1 or -1. So the product in the left hand side is equal to $\mathrm{KM}(X)$ and it will not change if we replace the pfaffians in it by their signs. Hence, we arrive at

$$\mathrm{KM}(X) = \prod_{x \in X^\tau} \mathrm{sgn}\,(\mathrm{pf}[w(x)]) = (-1)^{\mathrm{ind}_t w}.$$