On the existence of magnetic time reversal symmetry

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Outline

1. Introduction to time reversal symmetry in quantum mechanics
2. An application to the solid state physics
3. Deformation of time reversal symmetry: magnetic time reversal symmetry

Main references

[1] G. Panati, *Triviality of Bloch and Bloch-Dirac bundles*, Annales Henri Poincaré 8 (5), 995-1011, 2007.

[2] G. Panati, A. Pisante, *Bloch bundles, Marzari-Vanderbilt functional and maximally localized Wannier functions*, Communications in Mathematical Physics 322 (3), 835-875.

[3] D. Monaco, G. Panati, *Symmetry and Localization in Periodic Crystals: Trivialit of Bloch Bundles with a Fermionic Time-Reversal Symmetry*, Acta Appl. Math, 2015.

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Introduction to time reversal symmetry

Consider dynamics under conservative force without the presence of magnetic fields

- Classical mechanics

  If $t \to x(t)$ is a solution to the Newton equation

  $$m\ddot{x} = -\nabla V$$

  then $t \to x(-t)$ is a solution too

- Quantum mechanics (spinless particle)

  If $t \to \psi(t) \in L^2(\mathbb{R}^3, \mathbb{C})$ is a solution to the Schrödinger equation

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Introduction to time reversal symmetry

- Actually the complex conjugation operator C is the time reversal operator for spin 0 particles whose state space il $L^2(\mathbb{R}^3, \mathbb{C})$
- Observe that C is an antiunitary operator meaning that it is antilinear, it preserves the inner product up to complex conjugation and it is surjective

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However these are properties of every time reversal operator in quantum mechanics

Time reversal operator

In general, in quantum mechanics time reversal symmetry is represented by an operator Θ such that

- Θ is antiunitary
- $\Theta^2 = \pm\mathbb{1}$

This second property is a consequence of the antiunitary one. What one would phisically expect for time reversal operator is that

$$\Theta^2 = e^{i\varphi}\mathbb{1} \quad \text{for some} \quad \varphi \in \mathbb{R}$$

But

$$\begin{aligned}\Theta^3 \quad &= \Theta^2\Theta = e^{i\varphi}\Theta \\ &= \Theta\Theta^2 = e^{-i\varphi}\Theta\end{aligned}$$

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Time reversal symmetry: some examples

1. For spin 0 particle time reversal operator acts in $L^2(\mathbb{R}^3) \otimes \mathbb{C}$ as

$$\Theta_0 = C$$

2. For spin $\frac{1}{2}$ particle, time reversal operator acts in $L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$ as

$$\Theta_{1/2} = C \otimes e^{-i\pi S_y}$$

where $S = (S_x, S_y, S_z)$ is the spin operator and $S_y = \frac{1}{2}\sigma_y$

Notice that $\Theta_{1/2}^2 = -\mathbb{1}$

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An application to solid state physics

Suppose to consider a mesoscopic quantum system such that the Fermi energy lies in a gap (e.g. in insulators and semiconductors) and suppose that the system is macroscopically periodic with respect to the Bravais lattice

$$\Gamma = \mathrm{Span}_{\mathbb{Z}}\{e_1, \cdots, e_d\} \cong \mathbb{Z}^d \qquad d = 2, 3$$

1. In $\mathcal{H} = L^2(\mathbb{R}^d)$ consider the magnetic periodic Schrödinger operator (spin 0)

$$H^0_\Gamma = \frac{1}{2}(-i\nabla + A_\Gamma)^2 + V_\Gamma$$

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Bloq-Floquet(-Zak) transform

- In both cases H^s_Γ $(s = 0, 1/2)$ commutes with the translation on the Bravais lattice. Thus we can use the Bloch-Floquet tansform $\mathcal{U}_{BF}$ in order to write H^s_Γ as a fibered operator. We then obtain

$$\mathcal{U}_{BF} H^s_\Gamma \mathcal{U}_{BF}^{-1} = \int_{\mathbb{B}}^{\oplus} H^s_\Gamma(k) dk \ \text{ in } \ \mathcal{H}_\tau \cong L^2(\mathbb{B}, \mathcal{H}_f) \cong \int_{\mathbb{B}}^{\oplus} \mathcal{H}_f \, dk$$

  Example:

  $H^0_\Gamma(k) = \frac{1}{2}(-i\nabla_y + A_\Gamma(y) + k)^2 + V_\Gamma(y)$ acts in $\mathcal{D} = W^{2,2}(\mathbb{T}_Y) \subset \mathcal{H}_f$

- Each fiber operator $H(k)$ is self-adjoint and the pure point spectrum accumalates at infinity.

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Bloch bands and Fermi projectors

- We can label the eigenvalues of H^s_Γ increasing and repeated according to their multiplicity and consider the set of m Bloch bands:

$$\sigma_*(k) = \{E_i(k) \text{ s.t. } n \le i \le n+m-1\}$$

and assume they are separated by a gap from the rest of the spectrum

- Let $P_*(k) \in \mathcal{B}(\mathcal{H}_f)$ be the spectral projector corresponding to the set $\sigma_*(k) \subset \mathbb{R}$. The family of projectors $\{P_*(k)\}_{k\in\mathbb{R}^d}$ has the following properties:

(P1) the map $k \to P_*(k)$ is smooth from $\mathbb{R}^3$ to $\mathcal{B}(\mathcal{H}_f)$ (equipped with the operator norm)

(P2) the map $k \to P_*(k)$ is τ-covariant:

$$P(k+\lambda) = \tau(\lambda)P_*(k)\tau(\lambda)^{-1} \quad \forall k \in \mathbb{R}^3, \lambda \in \Lambda$$

where τ is a unitary representation of the the dual lattice to the Bravais one acting as $(\tau(\lambda)\varphi)(y) = e^{i\lambda\cdot y}\varphi(y)$

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Consequences of the existence of time reversal symmetry

In the case $A_\Gamma = 0$ ($\Rightarrow B_\Gamma = 0$) the Γ-periodic Hamiltonian is such that

$$[H_\Gamma, \Theta] = 0 \Rightarrow \Theta_f H_\Gamma(k)\Theta_f^{-1} = H_\Gamma(-k)$$

and the Fermi projectors satisfy also another property

$$(P3) \qquad \Theta_f P_*(k)\Theta_f^{-1} = P_*(-k)$$

This implies the triviality of Bloch Bundle and it is equivalent to the existence of a smooth and τ-equivariant Bloch frame.

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Magnetic time reversal symmetry

- Observe that $[H^s_\Gamma, \Theta] \neq 0$ because of the presence of a magnetic field. We are now going to look for a modified time reversal symmetry

- We are going to show a general Theorem not only for H^s_Γ ($s = 0, \frac{1}{2}$) but also for the same operators without taking into account the periodicity:

$$H^0 = \sum_{j=1}^{3} (P_j + A_j)^2 + V \qquad \text{(spinless particle)}$$

or

$$H^{1/2} = \sum_{j=1}^{3} (P_j + A_j)^2 + \frac{\sigma}{2} \cdot B + V \quad \text{(spin 1/2 particle)}$$

From now on H could be H^0 or $H^{1/2}$.

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Magnetic time reversal operator

Definition (Magnetic time reversal symmetry)

The Hamiltonian operator H is magnetic time reversal symmetric if there exists an operator T such that

- T is antiunitary (i.e. $T = UC$, U unitary, C complex conjugation) and its unitary part is a multiplication operator (i.e. $(U\psi)(x) = \mathcal{U}(x)\psi(x)$)
- $T^2 = \pm\mathbb{1}$
- $[H, T] = 0$

The operator T is called magnetic time reversal operator.

Does a magnetic time reversal operator really exist?

We want to prove the following

Theorem

The Hamiltonians H^0 or $H^{1/2}$ are magnetic time reversal symmetric if and only if the magnetic field associated to the vector potential A is null.

- We are going to give a sketch of the proof for $H^{1/2}$. In this case we have that $T^2 = -\mathbb{1}$ so T acts on $L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$ as

$$T = UC = \begin{pmatrix} 0 & \tau C \\ -\tau C & 0 \end{pmatrix}$$

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Sketch of the proof

(1) We can write $H^{1/2} = \frac{1}{2}\mathcal{D}^2 + V$ where $\mathcal{D} = \sigma \cdot (-i\nabla + A)$

(2) Because of V is any real-valued potential

$$[T, H^{\frac{1}{2}}] = 0 \Leftrightarrow [T, \mathcal{D}^2] = 0$$

(3) One can show that

$$[T, \mathcal{D}^2] = 0 \Leftrightarrow [\tau, P_j] = 2A_j\tau \quad \forall j = 1, 2, 3$$

(4) The previuos condition explicitly reads

$$\partial_j\tau = 2iA_j\tau, \qquad |\tau(x)| = 1$$

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(5) Notice that the 1-form on the l.s.h. of $\tau^{-1}d\tau = 2iA$ is closed. Thus if a solution exists the form A must be closed, yielding $B = 0$.

Viceversa if $B = 0$ then A is closed and it follows that $A = d\phi$ for a suitable function $\phi : \mathbb{R}^3 \to \mathbb{R}$.

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Viceversa if $B = 0$ then A is closed and it follows that $A = d\phi$ for a suitable function $\phi : \mathbb{R}^3 \to \mathbb{R}$.
Thus the solution to $\tau^{-1}d\tau = 2iA$ is exhibited by

$$\tau(x) = \tau(0)e^{2i(\phi(x)-\phi(0))}$$

We obtain that

$$[T, \mathcal{D}^2] = 0 \Leftrightarrow B = 0$$

What happens in the presence of a constant magnetic field?

If there is also a constant magnetic field $B = (0, 0, \beta)$, then one has to study

$$H^{1/2}_{\Gamma,\beta} = \frac{1}{2}(P + \frac{1}{2}(\beta e_3 \wedge x) + A_\Gamma)^2 + \frac{\sigma_3}{2}\beta + \frac{\sigma}{2} \cdot B_\Gamma + V_\Gamma$$

The main problem in order to replicate the prevoius strategy is that $[H^{1/2}_{\Gamma,\beta}, T_\Gamma] \neq 0$. To solve this problem one can replace T_Γ with the magnetic translation

$$T^\beta_\Gamma := e^{i\langle A_\beta, \gamma\rangle} T_\gamma$$

and enlarge the periodicity lattice. One has also to define the magnetic Bloch-Floquet transform from the Bloch-Floquet transform simply replacing T_Γ with T^β_Γ.

Obviously also in this case we have that $[H^{1/2}_{\Gamma,\beta}, T] \neq 0$.

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Thank you for the attention!