Discrete Symmetries in Crystals and Their Consequences

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Symmetry is a fundamental and profound concept in modern physics. As a rapidly developing field, topological states in solids have attracted much attention of both experimental and theoretical physicists due to their fancy properties and potential applications. In this note, we concentrate on the consequences led by various symmetries in crystals, or more specifically, these consequences of interest are exactly the symmetry protected topological states in the single electron picture. we briefly review some significant results of symmetry operations, and then the physical consequences constrained by each symmetry or their compositions are discussed.

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1. Time-reversal $\mathcal T$

1 1

 $1\\2\\2$

2 2 2

2 2 2

2

 $\frac{2}{2}$ $\frac{2}{2}$

2

2

Time-reversal symmetry is defined as

$$\mathcal{T}\hat{r}\mathcal{T}^{-1} = \hat{r}, \ \mathcal{T}\hat{p}\mathcal{T}^{-1} = \hat{p}, \tag{1}$$

and when a system is time-reversal invariant, we mean that

$$\mathcal{T}\hat{H}(\hat{\boldsymbol{r}}, \hat{\boldsymbol{p}})\mathcal{T}^{-1} = \hat{H}(\hat{\boldsymbol{r}}, -\hat{\boldsymbol{p}}). \tag{2}$$

Then, the canonical commutation relation $[\hat{r}, \hat{p}] = i\hbar$ under time-reversal requires that

I. A LITTLE BIT OF DISCRETE SYMMETRIES IN CRYSTALS

A. Local Symmetries

In the context of particle physics, namely, particles in vaccum, symmetries can be didived as local and global, or spacatime and gauge.

$$\mathcal{T}[\hat{\boldsymbol{r}}, \hat{\boldsymbol{p}}]\mathcal{T}^{-1} = \mathcal{T}(\hat{\boldsymbol{r}}\hat{\boldsymbol{p}} - \hat{\boldsymbol{p}}\hat{\boldsymbol{r}})\mathcal{T}^{-1} = \mathcal{T}(\hat{\boldsymbol{r}}\hat{\boldsymbol{p}} - \hat{\boldsymbol{p}}\hat{\boldsymbol{r}})\mathcal{T}^{-1}$$

$$= -\hat{\boldsymbol{r}}\hat{\boldsymbol{p}} + \hat{\boldsymbol{p}}\hat{\boldsymbol{r}} = -[\hat{\boldsymbol{r}}, \hat{\boldsymbol{p}}] = -i\hbar,$$
(3)

that is to say, time-reversal operator is commutative with imaginary unit, $[\mathcal{T},i]=0$. Due to the Wigner's theorem, any physical operator in Hilbert space must be either unitart or anti-unitary, \mathcal{T} have to be a anti-unitary operator satifying $\mathcal{T}=U\mathcal{K}$, where U is an unitary operator and \mathcal{K} is the complex conjugate operator.

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- 2. Particle-hole $\mathcal C$
- 3. Chiral ${\cal S}$

B. Point Group Symmetries

- 1. Discrete Translation T
- 2. Space Inversion ${\cal P}$
- 3. Mirror Reflection ${\mathcal M}$
- 4. Rotation C_n

C. Non-symmorphic Symmetries

- 1. Screw Axes and Glide Planes
- 2. Bands Sticking Together Effect

II. SYMMETRY PROTECTED TOPOLOGICAL INSULATORS

- A. Dirac Equation and the Invariants
- B. \mathcal{T}/\mathcal{S} -invariant

III. SYMMETRY PROTECTED TOPOLOGICAL SEMIMETALS

- A. Semimetals with Higher Degenerate Points
- 1. Dirac Semimetal
- 2. Unconventional Fermions
- **B. Nodal Line Semimetals**
- 1. T + P-invariant
- 2. \mathcal{M} -invariant
- 3. Screw-invariant
- C. Nodal Surface Semimetals
- 1. $\mathcal{T} + \mathcal{P} + \mathcal{M}$ -invariant
- IV. CONCLUSIONS AND OUTLOOKS