Symmetry and Point Group

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Outline

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Axial vector (pseudovector 赝矢量)

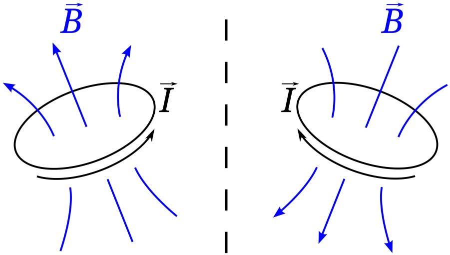
Define a vector as:

$$\mathbf{c} = \mathbf{a} \times \mathbf{b}$$

- $\mathbf{a}$ and $\mathbf{b}$ are polar vectors
- Under inversion: $\mathbf{a} \to -\mathbf{a}$, $\mathbf{b} \to -\mathbf{b}$

$$\mathbf{c} \to \mathbf{c}$$

Axial vector (pseudovector 赝矢量)



- A loop of wire carries a current $I \to$ magnetic field B
- Under a mirror plane: $I \to -I$
- Physical example: angular momentum $\mathbf{L} = \mathbf{r} \times \mathbf{p}$

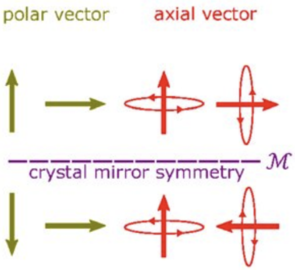
Axial vector (pseudovector 赝矢量)

Transformation rules:

$$\text{polar vector}: \mathbf{v}' = R\mathbf{v}$$
$$\text{pseudovector}: \mathbf{v}' = \det(R)R\mathbf{v}$$

- Physical examples of axial vector:
  magnetic field, angular momentum, angular velocity, torque

Axial vector (pseudovector 赝矢量)



A axial vector $\mathbf{a} = (a_x, a_y, a_z)$

- Inversion: $\to \mathbf{a}$
- Reflection $\mathcal{M}_x$: $\to (a_x, -a_y, -a_z)$

A polar vector $\mathbf{a} = (a_x, a_y, a_z)$

- Inversion: $\to -\mathbf{a}$
- Reflection $\mathcal{M}_x$: $\to (-a_x, a_y, a_z)$

Translation

Space translation

$$\mathbf{r} \to \mathbf{r} + \mathbf{a},$$

Time translation

$$t \to t + \tau$$

Translation

$$
\begin{aligned}
\mathsf{L}_{\mathbf{a}}\Psi(\mathbf{r}) &= \Psi(\mathbf{r}-\mathbf{a}) \\
&= \left(1 - a_i \frac{\partial}{\partial r_i} + \frac{1}{2} a_i a_j \frac{\partial^2}{\partial r_i \partial r_j}\right)\Psi(\mathbf{r}) \\
&= \exp\left(-a_i \frac{\partial}{\partial r_i}\right)\Psi(\mathbf{r}) \\
&= \exp\left(-\frac{i}{\hbar}\mathbf{a}\cdot\hat{\mathbf{p}}\right)\Psi(\mathbf{r})
\end{aligned}
$$

- The momentum operator $\hat{\mathbf{p}} = -i\hbar\nabla_{\mathbf{r}}$
- The space translation operator

$$
\mathsf{L}_{\mathbf{a}} = \exp\left(-\frac{i}{\hbar}\mathbf{a}\cdot\hat{\mathbf{p}}\right)
$$

- This is a unitary operator

Translation

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r}) = H\Psi(\mathbf{r})$$

- Act $\mathsf{L}_{\mathbf{a}}$ on both sides

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\mathsf{L}_{\mathbf{a}}\Psi(\mathbf{r}) &= \mathsf{L}_{\mathbf{a}}H\Psi(\mathbf{r}) \\ &= \mathsf{L}_{\mathbf{a}}H\mathsf{L}_{\mathbf{a}}^{-1}\mathsf{L}_{\mathbf{a}}\Psi(\mathbf{r}) \end{aligned}$$

- For a translation-invariant system, we have $[\mathsf{L}_{\mathbf{a}}, H] = 0$, thus

$$i\hbar\frac{\partial}{\partial t}\left[\mathsf{L}_{\mathbf{a}}\Psi(\mathbf{r})\right] = H\left[\mathsf{L}_{\mathbf{a}}\Psi(\mathbf{r})\right]$$

- $[\mathsf{L}_{\mathbf{a}}, H] = 0 \Longrightarrow [\hat{\mathbf{p}}, H] = 0$
- Momentum is a conserved quantity

Translation

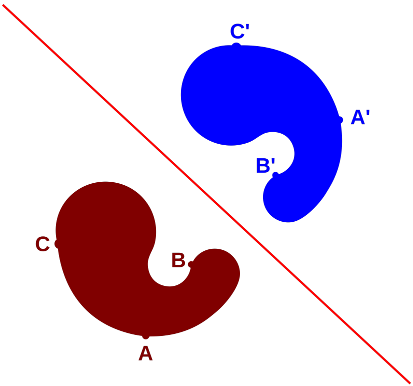
Time translation symmetry

Translation

Time translation symmetry

$\rightarrow$ Prove energy is conserved

Mirror (reflection)



- In 3D, the y-z plane reflection: $\mathcal{M}_x = \begin{pmatrix} -1 & & \\ & 1 & \\ & & 1 \end{pmatrix} \rightarrow \det(\mathcal{M}_x) = -1$
- For a polar vector

$$\mathbf{v} \rightarrow (-v_x, v_y, v_z)$$

Rotation

- The axis is a line of its fixed points

$$R_{\mathrm{r}}(\theta)\begin{pmatrix}x\\y\\z\end{pmatrix}=\begin{pmatrix}a & b & c\\d & e & f\\g & h & i\end{pmatrix}\begin{pmatrix}x\\y\\z\end{pmatrix}$$

- The matrix R is a memeber of 3D special orthogonal group $SO(3)\rightarrow\det(R)=1$
- In crystals, the ration angle $\theta=\frac{2\pi}{n}$

$$n=1,2,3,4,6$$

Rotation in crystallography

Assume

- $\mathbf{a}$ and $\vec{\mathbf{b}}$ are primitive vector of a 2D lattice
- $R(\theta)$ is rotation matrix

$$R(\theta)\mathbf{a} = m_{11}\mathbf{a} + m_{12}\mathbf{b}$$
$$R(\theta)\mathbf{b} = m_{21}\mathbf{a} + m_{22}\mathbf{b}$$

Write it with matrix form

$$\begin{pmatrix} \mathbf{a}' \\ \mathbf{b}' \end{pmatrix} = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \begin{pmatrix} \mathbf{a} \\ \mathbf{b} \end{pmatrix}$$

- Conclusion under primitive vector basis: If the rotation is a symmetry of a lattice, then all the elements of R are integers.
- The trace of any rotation matrix is invariant under any transform $\rightarrow$ $\mathrm{tr}(R)$ is interger

Rotation in crystallography

For a vector $\mathbf{a} = (x, y)^T$

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

- $\mathrm{tr}(R) = 2\cos\theta$ with $\theta = 2\pi/n$

$$\begin{aligned} \mathrm{tr}(R) &= 2, \quad n = 1 \\ \mathrm{tr}(R) &= -2, \quad n = 2 \\ \mathrm{tr}(R) &= -1, \quad n = 3 \\ \mathrm{tr}(R) &= 0, \quad n = 4 \\ \mathrm{tr}(R) &= 1, \quad n = 6 \end{aligned}$$

- We only have C_1, C_2, C_3, C_4, C_6 in crystals
- In 3D, $\mathrm{tr}(R) = 2\cos\theta + 1$

Inversion

$$\mathcal{P}\begin{pmatrix} x \\ y \\ z \end{pmatrix} \to \begin{pmatrix} -x \\ -y \\ -z \end{pmatrix}$$

- One fixed point: Inversion center

$$\det(\mathcal{P}) = -1$$

- Electric field: $\mathcal{P}\mathbf{E} = -\mathbf{E}$
- Magnetic field: $\mathcal{P}\mathbf{B} = \mathbf{B}$

Time reversal

$$t \to -t, \quad x \to x, \quad p \to -p$$

- Imaginary number: $i \to -i$

$$\begin{aligned} &[x, p] = i\hbar \\ \Longrightarrow &\mathcal{T}[x, p]\mathcal{T}^{-1} = \mathcal{T} i\hbar \mathcal{T}^{-1} \end{aligned}$$

- $\mathcal{T}$ is an anti-unitary operator

$$\mathcal{T} = U\mathcal{K}$$

where $\mathcal{U}$ is a unitary operator, and $\mathcal{K}$ is complex conjugation

- Anti-unitary properties

$$\mathcal{T}\psi = U\psi^*, \quad \langle \mathcal{T}\psi | \mathcal{T}\phi \rangle = (\langle \psi |)^* U^\dagger U (|\phi\rangle)^* = (\langle \psi | \phi \rangle)^* = \langle \phi | \psi \rangle$$

- In classical physics, we only have $\mathcal{T}^2 = +1$

Time reversal in spin-$1/2$ particle

Spin angular momentum reverse signs under $\mathcal{T}$:

$$\mathcal{T}\sigma_x\mathcal{T}^{-1} = -\sigma_x, \quad \mathcal{T}\sigma_y\mathcal{T}^{-1} = -\sigma_y, \quad \mathcal{T}\sigma_z\mathcal{T}^{-1} = -\sigma_z$$

- The operator can be represented by: $\mathcal{T} = i\sigma_y\mathcal{K}$

$$\begin{aligned}\mathcal{T}^2 = i\sigma_y\mathcal{K}i\sigma_y\mathcal{K} &= \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \\ &= \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} = -1\end{aligned}$$

Kramers degeneracy

For a time-reversal-invariant system, if $|\psi\rangle$ is an eigenstate of system, then $|\mathcal{T}\psi\rangle$ is also a eigenstate. For the case of $\mathcal{T}^2 = -1$, one has

$$\begin{aligned} \langle\psi|\mathcal{T}\psi\rangle &= \left\langle\mathcal{T}^2\psi\middle|\mathcal{T}\psi\right\rangle = -\langle\psi|\mathcal{T}\psi\rangle \\ \Longrightarrow \langle\psi|\mathcal{T}\psi\rangle &= 0 \end{aligned}$$

- ψ and $\mathcal{T}\psi$ are distinct states $\rightarrow$ Kramers doublet

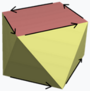
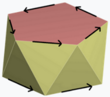
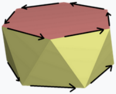
$$\psi_{n,\mathbf{k},\sigma} = \psi_{n,-\mathbf{k},-\sigma}$$

- At $k = 0$ or π, where $k = -k$, every single energy level is double degenerate

Improper rotaion

Also called rotation-reflection

Example polyhedra with rotoreflection symmetry

Group	S_4	S_6	S_8	S_{10}	S_{12}
Subgroups	C_2	C_3, $S_2 = C_i$	C_4, C_2	C_5, $S_2 = C_i$	C_6, S_4, C_3, C_2
Example	 beveled digonal antiprism	 triangular antiprism	 square antiprism	 pentagonal antiprism	 hexagonal antiprism

$\mathcal{PT}$ symmetry

$$\mathcal{P}: \mathbf{r} \to -\mathbf{r}, \quad \mathbf{k} \to -\mathbf{k}, \quad t \to t$$
$$\mathcal{T}: \mathbf{r} \to \mathbf{r}, \quad \mathbf{k} \to -\mathbf{k}, \quad t \to -t$$

For a Hamiltonian

$$\mathcal{PT} H(\mathbf{k}) (\mathcal{PT})^{-1} = H(\mathbf{k})$$

- $(\mathcal{PT})^2 = -1$, every energy band is doubly degeneracy

Transformations of H

Transformations: discrete and continuous

- Discrete transformations
  1. Reflection in mirror
  2. Interchange of two identical particles
  3. Charge conjugation (particles $\leftrightarrow$ anti-particles)
  4. Time reversal
- Continuous transformations
  1. Translation in time
  2. translation in space
  3. Rotation about an axis

$$\left|\psi'\right\rangle = \hat{U}(\alpha)\left|\psi\right\rangle$$

Unitary operator

The operator must be a unitary operator

$$
\begin{aligned}
&\langle\psi'|\psi'\rangle = \langle\psi|\psi\rangle = 1 \\
\rightarrow &\langle\psi|U^\dagger(\alpha)U(\alpha)|\psi\rangle = 1 \\
\rightarrow &U^\dagger(\alpha)U(\alpha) = 1
\end{aligned}
$$

Infinitesimal transformations

The operation of $U(\alpha)$ is equivalent to operating with n times of $U(\alpha/n) = u(\varepsilon)$

$$U(\alpha) = \lim_{n\to\infty} [U(\alpha/n)]^n = \lim_{n\to\infty} [U(\varepsilon)]^n$$

Thus, one can have

$$U(\varepsilon) = 1 - \frac{i\varepsilon}{\hbar} G$$

- G is a Hermitian operator
- G is called the generator of the transformation $\leftrightarrow$ physical observable

Infinitesimal transformations

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$$U(\alpha) = \lim_{n\to\infty} [U(\alpha/n)]^n = \lim_{n\to\infty} [U(\varepsilon)]^n$$

Thus, one can have

$$U(\varepsilon) = 1 - \frac{i\varepsilon}{\hbar} G$$

- Time translation operator

$$U_t(\varepsilon) = 1 - \frac{i\varepsilon}{\hbar} H$$

The generator is the Hamiltonian or energy operator, whose observable is what we identify classically as the energy of the system

Invariance, symmetry and conservation

- The physics is invariant under a transformation if

$$\begin{aligned}
&\big\langle \psi(t')\big|G\big|\psi(t')\big\rangle = \langle \psi(t)|G|\psi(t)\rangle \\
\Longrightarrow &\langle \psi(t)|U_t^\dagger G U_t|\psi(t)\rangle = \langle \psi(t)|G|\psi(t)\rangle \\
\Longrightarrow &U_t^\dagger G U_t = G \\
\Longrightarrow &[U, U_t] = 0
\end{aligned}$$

- The Hamiltonian is symmetric with respect to a transformation if

$$[U, H] = 0$$

- The observable associate with G is conserved if

$$[G, H] = 0$$

Invariance, symmetry and conservation

$$[U, U_t] = 0 \quad \Longleftrightarrow \quad [U, H] = 0 \quad \Longleftrightarrow \quad [G, H] = 0$$

invariance $\Longleftrightarrow$ symmetry $\Longleftrightarrow$ conservation

Find symmetries for H

In crystals, $\mathbf{k}$ is a godd quantum number

$$UH(\mathbf{k})U^\dagger = H(\mathcal{R}\mathbf{k})$$

- U is a unitary operator
- Transformation: $\mathbf{k}' = \mathcal{R}\mathbf{k}$

Find symmetries for H

$$H = v_F(\sigma_x k_x + \sigma_y k_y)$$

Mirror $\mathcal{M}_x$:

$$UH(k_x, k_y)U^\dagger = H(-k_x, k_y)$$

$$U = \sigma_y$$

Find symmetries for H

$$H = v_F(\sigma_x k_x + \sigma_y k_y)$$

Mirror $\mathcal{M}_y$:

$$UH(k_x, k_y)U^\dagger = H(k_x, -k_y)$$

$$U = \sigma_x$$

Find symmetries for H

$$H = v_F(\sigma_x k_x + \sigma_y k_y)$$

Inversion $\mathcal{I}$:

$$\mathcal{I} H(k_x, k_y) \mathcal{I}^\dagger = H(-k_x, -k_y)$$

$$\mathcal{I} = \sigma_z$$

Find symmetries for H

$$H = v_F(\sigma_x k_x + \sigma_y k_y)$$

Time reversal:

$$\mathcal{T} H(k_x, k_y) \mathcal{T}^\dagger = H(-k_x, -k_y)$$

$$\mathcal{T} = U\mathcal{K}, \quad U = -i\sigma_y$$

Find symmetries for H

$$H = v_F(\sigma_x k_x + \sigma_y k_y)$$

Particle-hole symmetry:

$$\mathcal{P}H(k_x, k_y)\mathcal{P}^\dagger = -H(-k_x, -k_y)$$

$$\mathcal{P} = U\mathcal{K}, \quad U = \sigma_x$$

Chiral symmetry:

$$\mathcal{C}H(k_x, k_y)\mathcal{C}^\dagger = -H(k_x, k_y)$$

Clearly, $\mathcal{C} = \mathcal{P}\mathcal{T}$

Find symmetries for H

$$H = v_F(\sigma_x k_x + \sigma_y k_y)$$

Rotation:

$$\mathbf{k}' = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} k_x \\ k_y \end{pmatrix}$$

The unitary operator

$$U(\theta) = e^{-i\frac{\theta}{2}\sigma_3}$$

The Hamiltonian satisfies

$$U(\theta)H(\mathbf{k})U^\dagger = H(\mathbf{k}')$$

Find symmetries for H

$$H = wk_x + v_F(\sigma_x k_x + \sigma_y k_y)$$

- Mirror $\mathcal{M}_y$
- Particle-hole symmetry
- Rotation C_{2x}
- $\mathcal{M}_x \mathcal{T}$

Outline

Group

$$(G, *)$$

- Set: $\{g_1, g_2, \dots\}$
- Operation $*$

Group

Group

$$(G, *)$$

- Set: $\{g_1, g_2, \dots\}$
- Operation $*$

Algebra

$$(G, *, +)$$

Group

- Identity element

$$e * a = a * e = a$$

- Associativity

$$(a * b) * c = a * (b * c)$$

- Inverse element
  For every element $a \in G$, there exists an inverse element $a^{-1} \in G$

$$a * a^{-1} = a^{-1} * a = e$$

- Closure

$$\forall a, b {\in} G, , \quad a * b \in G$$

5 C_n

- C_1
- C_2
- C_3
- C_4
- C_6

5 C_{nh}

- C_{1h}
- C_{2h}
- C_{3h}
- C_{4h}
- C_{6h}

4 C_{nv}

- C_{2v}
- C_{3v}
- C_{4v}
- C_{6v}

3 S_{2m}

- S_2
- S_4
- S_6

4 D_n

- D_2
- D_3
- D_4
- D_6

4 D_{nh}

- D_{2h}
- D_{3h}
- D_{4h}
- D_{6h}

2 D_{nd}

- D_{2d}
- D_{3d}

5 Cubic point group

- T
- T_d
- T_h
- O
- O_h

Conclusion

- Transformation in system
- Symmetry and invariant