Qin’s seminar

--- teaching part

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2022. 9. 30

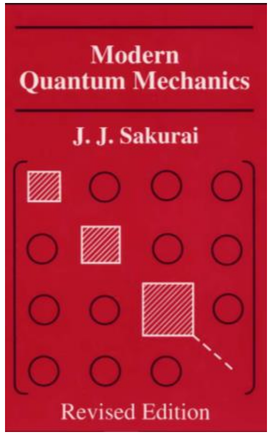
Time reversal Θ

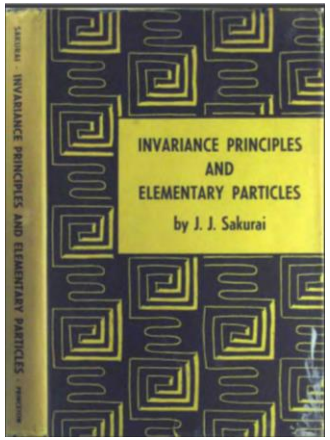
- Refs: P277 《群论及其在固体物理中的应用》
  P103 《quantum field theory in a nutshell》, A. Zee
  曾谨言，第九章 时间反演

。。。。。。。。。。

Most inspiring demonstration:

J. J. Sakurai(Jun John, 1933-1982)





《Modern quantum mechanics》

《Invariance principle and elementary particles》

时间倒流了吗？

你不在的时候，我有个机会去过了一段年轻时候的日子。
本来以为我再活一次的话，也许会有什么不一样，结果，
还是差不多，没什么不同。只是突然觉得，再活一次的话，
好像真的没那个必要，真的没那个必要。

你知道我以后想做什么吗？
我要去告诉别人他们不知道的事，
给别人看他们看不到的东西，我想，
这样一定天天都很好玩。

《 A one and a Two 》： 杨德昌 的 《一一》

Learning to teaching

- Wigner（1932）: “时间反演态”并不意味着“time reversal”

  → misnomer, “science fictions”

  而是“reversal of direction of motion”

时间反演对称性（反线性）并不导致某种守恒量

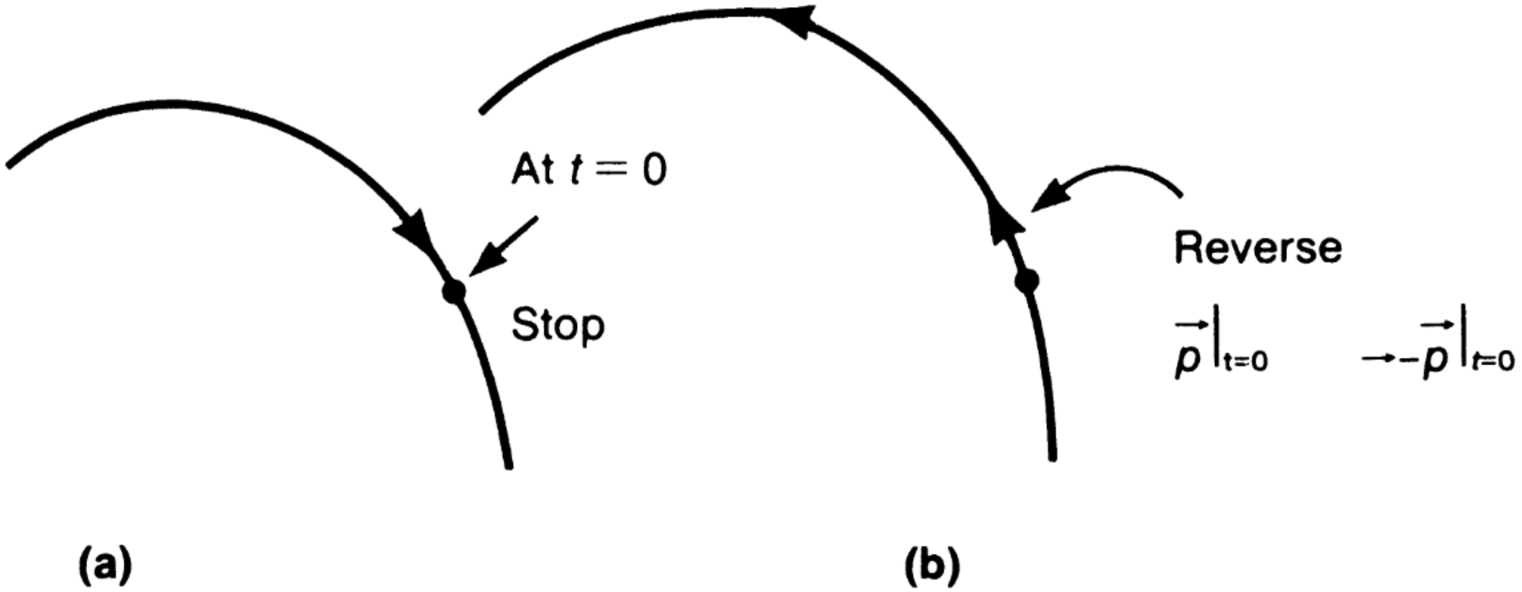


FIGURE 4.9. (a) Classical trajectory which stops at $t = 0$ and (b) reverses its motion $\mathbf{p}|_{t=0} \rightarrow -\mathbf{p}|_{t=0}$.

Newtonian mechanics

$$m\frac{d^2\vec{x}}{dt^2} = \vec{F}(\vec{x})$$

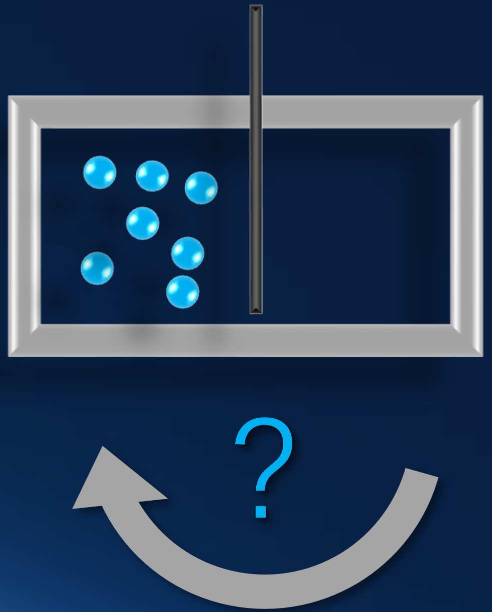
Clearly if $\vec{x}(t)$ is a possible trajectory, then likewise so is $\vec{x}(-t)$ since

$$m\frac{d^2\vec{x}}{d(-t)^2} = \vec{F}(\vec{x})$$

Falling body vs thrown upwards

覆水难收

未来与过去不同



气体的等温自由膨胀：不可逆性

Q：微观上每个气体分子运动可逆，为什么宏观上无法退回到膨胀前？

Wigner(1932,1959): out of dilemma

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t)=\hat{H}\psi(\vec{r},t)$$

$$\psi(\vec{r},t)=e^{i(\vec{p}\cdot\vec{x}-E_n t)/\hbar} \qquad t\rightarrow -t \qquad \psi(\vec{r},t)=e^{i(\vec{p}\cdot\vec{x}+E_n t)/\hbar}$$

- Contradiction: $\frac{p^2}{2m}\psi(\vec{r},t)=E_n\psi(\vec{r},t)$ $\qquad$ $\frac{p^2}{2m}\psi(\vec{r},t)=-E_n\psi(\vec{r},t)$

Introduce time reversed state $\qquad \Theta\psi(\vec{r},t)\overset{\text{def}}{=}$

$$e^{-i(\vec{p}\cdot\vec{x}-E_n(-t))/\hbar}=e^{i(-\vec{p}\cdot\vec{x}-E_n t)/\hbar}$$

$\Theta\ |p\rangle=|-p\rangle$, E_n keep invariant!

- We require the probability of finding a particle which will be the same .

$\langle\psi|\psi\rangle = \langle\Theta\psi|\Theta\psi\rangle$

We have two choices : $|\langle\varphi|\psi\rangle| = |\langle\Theta\varphi|\Theta\psi\rangle|$

$\langle\varphi|\psi\rangle = \langle\Theta\varphi|\Theta\psi\rangle$ (Θ unitary, keep inner product invariant)

$\langle\varphi|\psi\rangle^* = \langle\psi|\varphi\rangle = \langle\Theta\varphi|\Theta\psi\rangle$ (Θ anti-unitary: an extra complex conjugate)

Hermitian operator

➡ a generalization of a real number

Hermitian conjugate of $|\psi\rangle$

$|\psi\rangle^{\dagger} = \langle\psi|$

$\langle\psi|^{\dagger} = |\psi\rangle$

Why this requirement $\hat{O} = \hat{O}^{\dagger}$ (Hermitian, or self-adjoint) ?

$a = \langle\psi|\hat{O}|\psi\rangle = \langle\psi|\hat{O}^{\dagger}|\psi\rangle = a^{*}$ (physical observable)

Generally, $\langle\varphi|\hat{O}|\psi\rangle = \langle\psi|\hat{O}|\varphi\rangle^{*}$

反线性幺正算符Θ

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t)=\hat{H}\psi(\vec{r},t)$$

数学处理：$t\rightarrow -t$

$\mathrm{i}\hbar\frac{\partial\psi(\vec{r},-t)}{\partial(-t)}=H\psi(\vec{r},-t)$，不满足薛定谔方程
等式两边取复共轭，发现

当$\psi'(\vec{r},t)=\psi^*(\vec{r},-t)$满足薛定谔方程，
回到对于时间反演算符Θ(物理)的要求，将时间反演算符作用于方程的两边

$$\Theta\mathrm{i}\hbar\frac{\partial\psi(\vec{r},t)}{\partial(t)}=\Theta H\psi(\vec{r},t)$$

如果$\Theta=UK$是反线性的幺正算符，问题迎刃而解，Θ与i的对易关系负号合并数学上$t\rightarrow -t$的要求。

左边$=-\mathrm{i}\hbar\Theta\frac{\partial\psi(\vec{r},t)}{\partial(t)}=$右边$=H\Theta\psi(\vec{r},t)$

$$\left[\Theta, i\frac{\partial}{\partial t}\right] = 0 \text{ match } [\Theta, H] = 0$$

如果 $\Theta\psi(\vec{r},t) = \psi^*(\vec{r},-t)$

一切变得简单，复共轭视为打补丁（**qinsx**）

得到$\psi^*(\vec{r},-t)$满足薛定谔方程的形式。

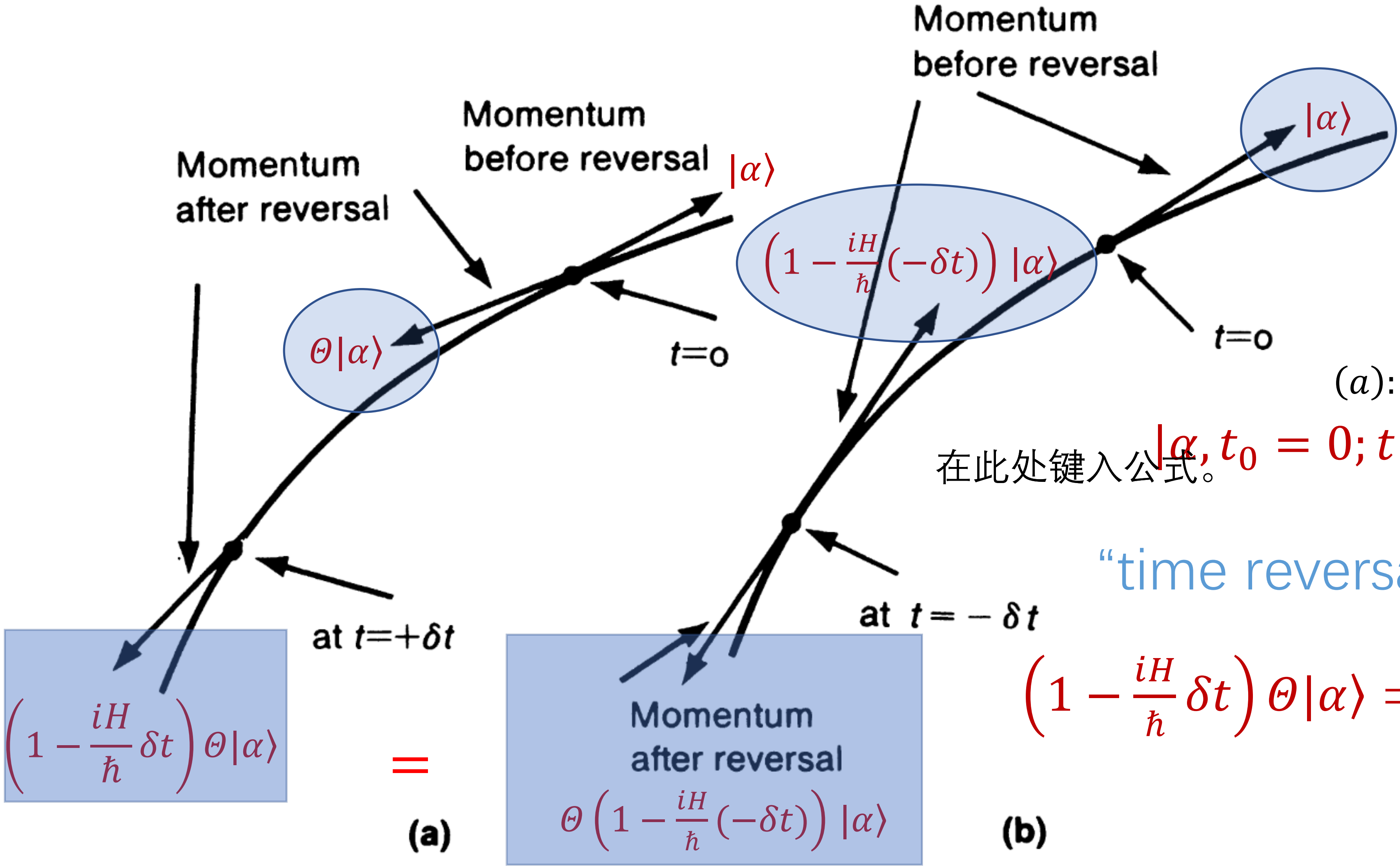


FIGURE 4.11. Momentum before and after time reversal at time $t=0$ and $t=\pm\delta t$.

Note:

All the treatments start at $t=0$

(a): $0\rightarrow\delta t$

在此处键入公式。

$$|\alpha, t_0=0; t=\delta t\rangle = \left(1-\frac{iH}{\hbar}\delta t\right)|\alpha\rangle$$

"time reversal symmetry " requires

$$\left(1-\frac{iH}{\hbar}\delta t\right)\Theta|\alpha\rangle = \Theta\,|\alpha, t_0=0; t=-\delta t\rangle$$

$$= \Theta\left(1-\frac{iH}{\hbar}(-\delta t)\right)|\alpha\rangle$$

(b): $(-\delta t\rightarrow 0)^{-1}$

"reversal of motion"

$$\left(1-\frac{iH}{\hbar}\delta t\right)\Theta|\alpha\rangle = \Theta\left(1-\frac{iH}{\hbar}(-\delta t)\right)|\alpha\rangle$$

$$-iH\Theta = \Theta iH$$

If Θ is unitary,

$$-H\Theta = \Theta H$$

$$H\Theta|n\rangle = -\Theta H|n\rangle = -E_n\Theta\,|n\rangle$$

Nonsensical!

Θ is anti-unitary $\rightarrow$ antilinear

$$-iH\Theta = \Theta iH = -i\Theta H$$

$$H\Theta = \Theta H$$

时间反演算符的性质

- 反线性

$$\Theta(a\phi + b\varphi) = a^*\Theta\phi + b^*\Theta\varphi$$

$$(\Theta\phi, \Theta\varphi) = (\varphi, \phi) = (\phi, \varphi)^*$$

- 反幺正（反线性的幺正）

$$\Theta = UK$$

Unitary * complex conjugate

The operation of time-reversal operator

$$\langle\beta|\Theta|\alpha\rangle = \langle\beta|(\Theta|\alpha\rangle)$$

$$|\tilde{\alpha}\rangle = \Theta|\alpha\rangle, \qquad |\tilde{\beta}\rangle = \Theta|\beta\rangle,$$

Dual Corres-pondence

$proof$:

$$|\gamma\rangle \equiv \otimes^{\dagger}|\beta\rangle$$

$$|\gamma\rangle \leftrightarrow \langle\gamma| = \langle\beta|\otimes$$

$$\langle\beta|\otimes|\alpha\rangle = \langle\gamma|\alpha\rangle = \langle\tilde{\alpha}|\tilde{\gamma}\rangle$$

$$= \langle\tilde{\alpha}|\Theta\otimes^{\dagger}|\beta\rangle$$

$$= \langle\tilde{\alpha}|\Theta\otimes^{\dagger}\Theta^{-1}\Theta|\beta\rangle$$

$$= \langle\tilde{\alpha}|\Theta\otimes^{\dagger}\Theta^{-1}|\tilde{\beta}\rangle$$

Identity from the antiunitary nature of Θ

$$\langle\beta|\otimes|\alpha\rangle = \langle\tilde{\alpha}|\Theta\otimes^{\dagger}\Theta^{-1}|\tilde{\beta}\rangle$$

Linear operator

Odd/even operator

$$\Theta A\Theta^{-1} = \pm A$$

For Hermitian observables:

$$\langle\beta|A|\alpha\rangle = \langle\tilde{\alpha}|\Theta A\Theta^{-1}|\tilde{\beta}\rangle$$

$$\langle\beta|A|\alpha\rangle = \pm\langle\tilde{\beta}|A|\tilde{\alpha}\rangle^{*}$$

- Expectation value

$$\langle\alpha|p|\alpha\rangle = -\langle\tilde{\alpha}|p|\tilde{\alpha}\rangle$$

$$\Theta p \Theta^{-1} = -p$$

$$p\Theta\,|\mathrm{p}'\rangle = -\Theta p|p'\rangle = -\Theta p'|p'\rangle = -p'\Theta|p'\rangle$$

$\Theta\,|p'\rangle = |-p'\rangle$ (up to a phase factor): $|-p'\rangle$ is the momentum eigen-ket with eigenvalue $-p'$

$$\langle\alpha|x|\alpha\rangle = \langle\tilde{\alpha}|x|\tilde{\alpha}\rangle$$

$$\Theta x \Theta^{-1} = x$$

$$\Theta\,|x'\rangle = |x'\rangle \text{ (up to a phase)}$$

- Check the fundamental commutation relation：

$$[x_i, p_j]|\quad\rangle = i\hbar\delta_{ij}\,|\quad\rangle$$

$$\Theta\,[x_i, p_j]\Theta^{-1}\Theta|\quad\rangle = \Theta i\hbar\delta_{ij}\,|\quad\rangle$$

$$[x_i, -p_j]\Theta|\quad\rangle = -i\hbar\delta_{ij}\Theta\,|\quad\rangle$$

for angular-momentum operator,

$$[J_i, J_j] = i\hbar\varepsilon_{ijk}J_k$$

$$\Theta J\Theta^{-1} = -J$$

- This is consistent for spin-less system where $J = r \times p$

Wave function

$|\alpha\rangle$: a spinless single − particle state

$$|\alpha\rangle = \int d^3x' \, |x'\rangle\langle x'|\alpha\rangle$$

$$\Theta|\alpha\rangle = \int d^3x' \, |x'\rangle\langle x'|\alpha\rangle^*$$

$$\psi(x') \rightarrow \psi^*(x')$$

$\boldsymbol{Theorem}$: Suppose the Hamiltonian is invariant under time reversal and the energy eigen-ket $|n\rangle$ is nondegenerate; then the corresponding Energy eigen-fuction is real (or ,more generally, a real function times a phase factor independent of $\boldsymbol{x}$)

$$\langle x'|n\rangle = \langle x'|n\rangle^*$$

The eigen-spinor of $\sigma \cdot \hat{n}$

$$\sigma \cdot \hat{n}\mathcal{X} = \mathcal{X}$$

$\hat{n} \rightarrow$ unit vector,

polar angle: β ; azimuthal angle: α

$$\sigma = (\sigma_x, \sigma_y, \sigma_z)$$

$$\hat{n} = (\cos\beta\cos\alpha, \cos\beta\sin\alpha, \sin\beta)$$

$$\mathcal{X} = \begin{pmatrix} \cos\left(\frac{\beta}{2}\right) e^{-i\alpha/2} \\ \sin\left(\frac{\beta}{2}\right) e^{-i\alpha/2} \end{pmatrix}$$

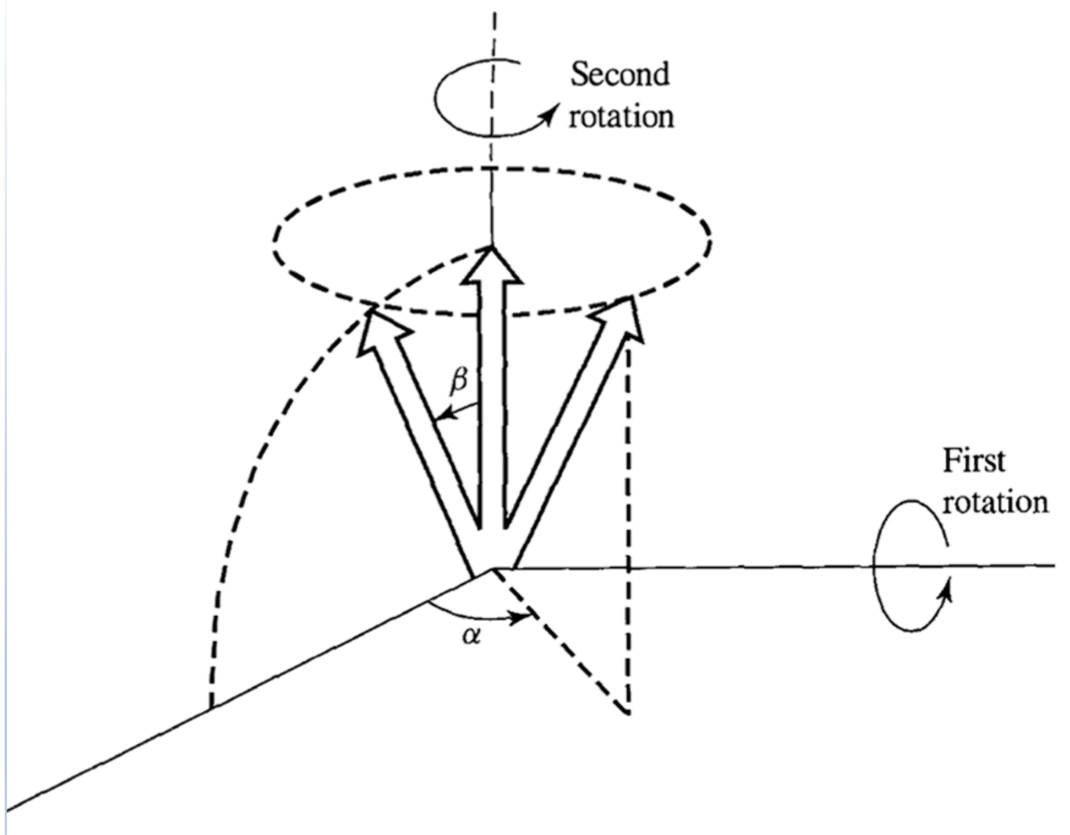


FIGURE 3.3 Construction of $\sigma \cdot \hat{\mathbf{n}}$ eigenspinor.

For spin-1/2 system

$$\sigma = \frac{2S}{\hbar}$$

$$\hat{n} = (0,0,1)$$

$$\sigma \cdot \hat{n} = \sigma_z$$

The first rotation, the operator : $e^{-iS_y\beta/\hbar}$

$|+\rangle$: $eigenvector\ of\ \sigma_z$

1: eigenvalue

The second rotation, the operator : $e^{-iS_z\alpha/\hbar}$

$$e^{-iS_z\alpha/\hbar}\, e^{-iS_y\beta/\hbar}|+\rangle = e^{-i\sigma_z\alpha/2}\, e^{-i\sigma_y\beta/2}|+\rangle$$

$$= \left[\cos\frac{\alpha}{2} - i\,\sigma_z \sin\frac{\alpha}{2}\right]\left[\cos\beta - i\,\sigma_y \sin\frac{\beta}{2}\right]\binom{1}{0}$$

$$= \begin{pmatrix} \cos\left(\frac{\beta}{2}\right)e^{-i\alpha/2} \\ \sin\left(\frac{\beta}{2}\right)e^{-i\alpha/2} \end{pmatrix}$$

Time reversal for a spin ½ system

- $|\hat{n};+\rangle = e^{-iS_z\alpha/\hbar}e^{-iS_y\beta/\hbar}\,|+\rangle$
- $\Theta\,|\hat{n};+\rangle = e^{-iS_z\alpha/\hbar}e^{-iS_y\beta/\hbar}\,\Theta\,|+\rangle = \eta\,|\hat{n};-\rangle$ (*)
- $|+\rangle$ is the initial state, the factor $e^{-iS_z\alpha/\hbar}e^{-iS_y\beta/\hbar}$ is the transformation of $|+\rangle$, Θ directly operates on $|+\rangle$, it is the requirement for TRS, we expect $|\hat{n};-\rangle$(compare to the argument in P271, (4.4.22-4.4.24)) ,

η stands for an arbitrary phase(a complex number of modulus unity)

$$|\hat{n};-\rangle = e^{-iS_z\alpha/\hbar}e^{-iS_y(\pi+\beta)/\hbar}\,|+\rangle$$

$$\Theta = UK$$

Identity

- $$\exp\left(-\frac{i\vec{\sigma}\cdot\vec{n}\alpha}{2}\right) = \left[1 - \frac{(\vec{\sigma}\cdot\vec{n})^2}{2!}\left(\frac{\alpha}{2}\right)^2 + \frac{(\vec{\sigma}\cdot\vec{n})^2}{4!}\left(\frac{\alpha}{2}\right)^4 - \cdots\right]$$
$$-i\left[(\vec{\sigma}\cdot\vec{n})\frac{\alpha}{2} - \frac{(\vec{\sigma}\cdot\vec{n})^3}{3!}\left(\frac{\alpha}{2}\right)^3 + \cdots\right]$$
$$= \mathbf{1}\cos\left(\frac{\alpha}{2}\right) - \boldsymbol{i}\,(\vec{\sigma}\cdot\vec{n})\sin\left(\frac{\alpha}{2}\right)$$

$$(\vec{\sigma}\cdot\vec{a})\left(\vec{\sigma}\cdot\vec{b}\right) = \vec{a}\cdot\vec{b} + i\,\vec{\sigma}\cdot\left(\vec{a}\times\vec{b}\right)$$

$$\left(\vec{\sigma}\cdot\vec{\hat{n}}\right)^n = \begin{cases} 1 & for\ n\ even \\ \vec{\sigma}\cdot\vec{\hat{n}} & for\ n\ odd \end{cases}$$

Time reversal for a spin ½ system

$$\Theta = \eta e^{-i\pi s_y/\hbar} K = -i\,\eta \frac{2S_y}{\hbar} K = -i\,\eta \sigma_y K$$

Then we can check $\Theta\,|\hat{n};+\rangle = e^{-is_z\alpha/\hbar} e^{-is_y\beta/\hbar}\,\Theta\,|+\rangle$

$$\Theta e^{-is_z\alpha/\hbar} = e^{-is_z\alpha/\hbar}\Theta \quad (1)$$

$$\Theta e^{-is_y\beta} = e^{-is_y\beta/\hbar}\Theta \quad (2)$$

In (1): $i \to -i, S_y\, S_z = -S_z\, S_y$
In (2): exponential factor
Is real. And S_y commute
with itself

- $\mathcal{X}(\hat{n};+) \text{ −> } |\hat{n};+\rangle$
- $\sigma\cdot\hat{n}\mathcal{X}(\hat{n};+) = \mathcal{X}(\hat{n};+)$, then
- $-i\sigma_y\mathcal{X}^*(\hat{n};+) \text{ −> } |\hat{n};-\rangle$
- Choosing S_z representation

$$e^{-i\pi S_y/\hbar}|+\rangle = +|-\rangle,\quad e^{-i\pi S_y/\hbar}|-\rangle = -\,|+\rangle$$

$$\Theta(c_+|+\rangle + c_-|-\rangle) = +\eta c_+{}^*|-\rangle - \eta c_-{}^*|+\rangle,$$
$$\Theta^2(c_+|+\rangle + c_-|-\rangle) = -|\eta|^2\, c_+|+\rangle - |\eta|^2 c_-|-\rangle$$
$$= -\,(c_+|+\rangle + c_-|-\rangle)$$

$\Theta^2 = -1 \rightarrow$ kramers degeneracy

证明:

$\because [\Theta, H] = 0, \qquad H\psi = E\psi, H\Theta\psi = E\Theta\psi,$
$\Theta\psi$与ψ对应同样的能量E。

假设$\Theta\psi = e^{i\alpha}\psi$（即两个波函数等价），则有
$\Theta^2\psi = \Theta e^{i\alpha}\psi = e^{-i\alpha}\Theta\psi = \psi \Rightarrow \Theta^2 = 1$
与$\Theta^2 = -1$相矛盾，故波函数不等价，二重简并。

The presence of K (complex conjugate) makes Θ "anti-linear unitary."

- Let $\Theta = UK$ $U^{-1}iU = i,$ U is the unitary operator.

(1) for a spinless particle (U: phase factor)

$$\Theta = K \Rightarrow \Theta^2 = 1$$

(2)odd number of electrons

$$\Theta = -i\sigma_2 K \Rightarrow \Theta^2 = -1$$

⬇

Kramers degeneracy

由于时间反演算符和哈密顿量对易，对系统作时间反演不会改变系统的能量，因此

$$E_n\left(\vec{k}\right)=E_n\left(-\vec{k}\right)$$

考虑倒空间中能带的周期性

$$E\left(\vec{k}\right)=E\left(\vec{k}+\vec{K}\right)$$

$\vec{K}$为倒格矢，考虑

$$E\left(\frac{\vec{K}}{2}-\delta\vec{k}\right)=E\left(-\frac{\vec{K}}{2}+\delta\vec{k}\right)=E\left(\frac{\vec{K}}{2}+\delta\vec{k}\right)$$

$E\left(\vec{k}\right)$是以零斜率进入布里渊区边界。

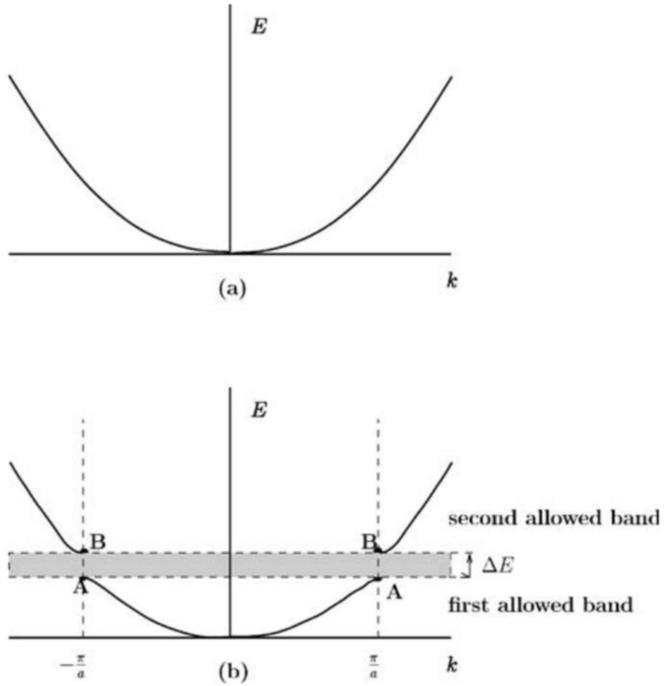
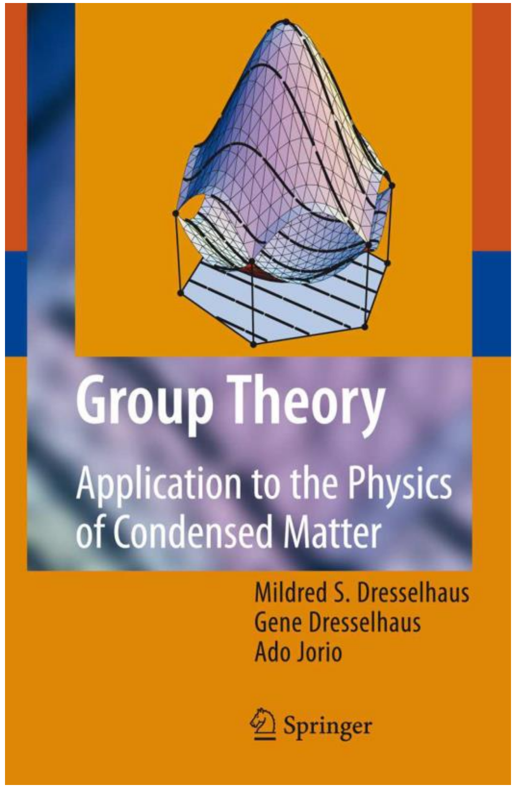


Fig. 16.1. Simple $E(\boldsymbol{k})$ diagram for a spinless electron illustrating both $E(\boldsymbol{k})=E(-\boldsymbol{k})$ and the zero slope of $E(\boldsymbol{k})$ at the Brillouin zone boundary



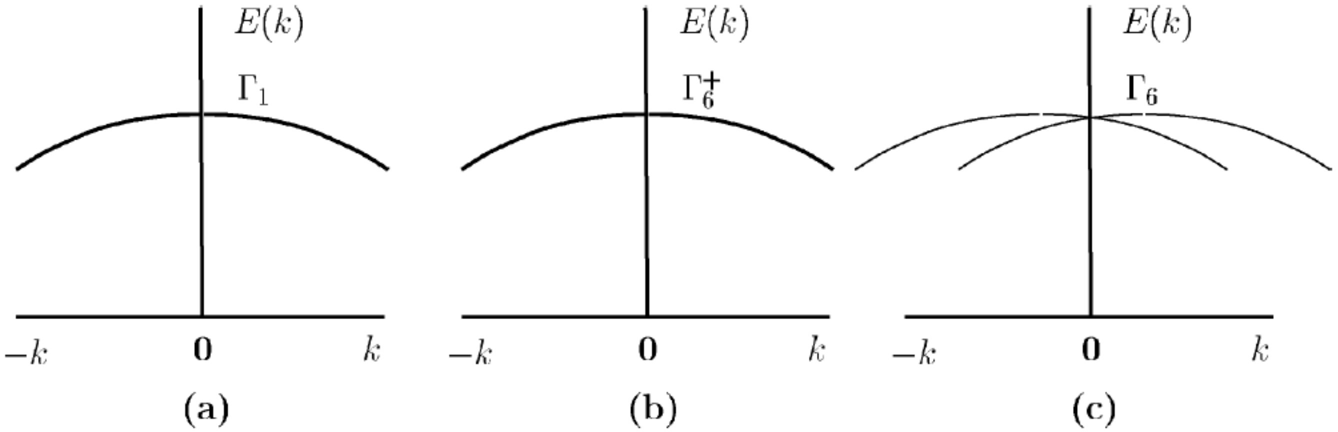


Fig. 16.2. Schematic example of Kramers degeneracy in a crystal in the case of: (**a**) no spin–orbit interaction where each level is doubly degenerate $(\uparrow, \downarrow)$, (**b**) both spin–orbit interaction and inversion symmetry are present and the levels are doubly degenerate, (**c**) spin–orbit interaction and no spatial inversion symmetry where the relations (16.23) and (16.24) apply

$$E_{n\uparrow}(\boldsymbol{k}) = E_{n\downarrow}(-\boldsymbol{k}) \tag{16.23}$$

$$E_{n\downarrow}(\boldsymbol{k}) = E_{n\uparrow}(-\boldsymbol{k})\,. \tag{16.24}$$

Back to wave mechanics

$$i\hbar \frac{\partial}{\partial t}\psi(\boldsymbol{x},t) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi(\boldsymbol{x},t)$$

$$\psi(\boldsymbol{x},t) = u_n(\boldsymbol{x})e^{-iE_nt/\hbar} \qquad \psi^*(\boldsymbol{x},-t) = u_n{}^*(\boldsymbol{x})e^{-iE_nt/\hbar}$$

If at $t = 0$ the wave function is given by

$\psi = \langle \boldsymbol{x}|\alpha\rangle$, then

$\Theta\psi = \langle \boldsymbol{x}|\alpha\rangle^*$

In the spin-less case

Variance or constant ? $t, \ \Delta t$

$$\Theta \frac{\partial}{\partial t}\psi = \Theta \frac{\psi(t+\Delta t)-\psi(t)}{\Delta t} = \frac{\psi^*(-t+\Delta t)-\psi^*(-t)}{\Delta t}$$

$$= -\frac{\psi^*\big(-(t-\Delta t)\big)-\psi^*(-t)}{-\Delta t} = -\frac{\partial\psi^*(-t)}{\partial t} = -\frac{\partial}{\partial t}\Theta\psi$$

$\Theta i = -i\Theta, \quad \Theta\frac{\partial}{\partial t} = -\frac{\partial}{\partial t}\Theta$ ⇒ $\left[\Theta, i\frac{\partial}{\partial t}\right] = 0$

$$\Theta\psi(\vec{r},t) = \psi^*(\vec{r},-t),$$

$\Theta e^{iHt}|\alpha\rangle = e^{iHt}\Theta\,|\alpha\rangle$ (here, $H\Theta = \Theta H$)

Kramers' theorem

which states that the energy levels of a time-reversal invariant system with an odd number of electrons are n-fold degenerate where n is even(偶数).

- Essentially the energy levels come in pairs of Kramers doublets, and you can only split these pairs by Hendrik Kramers (1894–1952) introducing a perturbation that breaks time-reversal, such as a magnetic field.

- 时间反演的灵魂是什么?

当$t \to -t$， 你希望什么保持不变? 薛定谔方程?
Ok，如果是，需要取复共轭，
这样产生了所谓的反线性幺正算符。

定义了state $|p, s\rangle$， 要求$\Theta|p, s\rangle = |-p, -s\rangle$，一切可以推导
时间在牛顿力学里是动力学变量，在Hilbert space不是。
从运动轨迹的反演 vs 态演化“轨迹”的反演

Learning to teaching

- 苔

作者： 袁枚（清代）

白日不到处，青春恰自来。
苔花如米小，也学牡丹开。

"The essence of education means that
one tree shakes another tree,
one cloud pushes another cloud,
and one soul awakens another soul."

----- German philosopher Karl Theodor Jaspers，《What is education》

Best way to learn is to learn from the best