Notes about Spin and TR Symmetry

Taper

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Abstract

This is a note about TR symmetry, with its application in the theory of condensed matter physics. The two reference book are the classic by Sakurai [1], and the other by Bernevig [2]. It contains a summary of treatment of Spin (actually, rotation) in quantum mechanics, which is needed to discuss the TR symmetry operator.

Contents

1 Review of Spin theory

Outline:

1. The representation of infinitesimal operator.
2. From traditional rotational operators to commutation relationship
3. From commutators to their eigenvalues.
4. Summarize some further results regarding the matrix representation of those operators.

1.1 The representation of transformation

To find an operator for a physical transformation, we naturally encounters the theory of representation of groups. Why groups? See the following notes for an bird view. (The note is an excerpt from my notes about Quantum Field Theory by Weinberg, which is still in its infancy because the book is so hard to read)

> The set of all symmetries transformations obviously can have a group structure. By giving each symmetry transformation a unitary or antiunitary operator, a representation of such group is obtained. However, such a representation can be projective (projective as in projective geometry, or $\mathbb{CP}^n$), since operators acts on ket spaces, which is already projective (i.e. within a freedom of phase).

Here I outlined one general procedure to obtain such representation from infinitesimal transformations. This procedure is discussed in chapter 1 and 2 of [1]. We first needs two thing to characterize a tranformation: a Hermitian operator G and an infinitesimal change ε. I am not sure about how to choose G, but I think the choice for ε should be clear. Here are three typical examples.

For displacement in x direction:

$$G \to \frac{p_x}{\hbar}, \varepsilon \to \mathrm{d}x \tag{1.1.1}$$

For an infinitesimal time evolution:

$$G \to \frac{H}{\hbar}, \varepsilon \to \mathrm{d}t \tag{1.1.2}$$

For infinitesimal rotation around k th axis:

$$G \to \frac{J_k}{\hbar}, \varepsilon \to \mathrm{d}\phi \tag{1.1.3}$$

Or more general (let the rotation be characterized by $\mathbf{J} \cdot \hat{\mathbf{n}}$, where $\hat{\mathbf{n}}$ is a unit vector), we have:

$$G \to \frac{\mathbf{J} \cdot \hat{\mathbf{n}}}{\hbar}, \varepsilon \to \mathrm{d}\phi \tag{1.1.4}$$

Here $\mathbf{J} = (J_x, J_y, J_z)$ is defined such that the substitution 1.1.3 indeed produces a rotation. What do we mean by "indeed" here? This will be explained in section 1.2.

Then the operator corresponding to the infinitesimal transformation is

$$U_\varepsilon = 1 - i\,G\varepsilon \tag{1.1.5}$$

And for a finite transformation (let Δ denotes the finite transformation):

$$\lim_{N\to\infty}\left[1 - iG\frac{\Delta}{N}\right]^N = \exp(-iG\Delta) \tag{1.1.6}$$

For example, in the case of rotation we have (using $\mathscr{D}$ to denote the operator):

$$\mathscr{D}(\hat{\mathbf{n}}, \mathrm{d}\phi) = 1 - i\frac{\mathbf{J}\cdot\hat{\mathbf{n}}}{\hbar}\,\mathrm{d}\phi \tag{1.1.7}$$

$$\mathscr{D}(z, \phi) = \exp\left(\frac{-iJ_z\phi}{\hbar}\right) \tag{1.1.8}$$

Note that, here G is regarded as a generator of physical transformation:

Table 1: Generators

Generator	Physically generated transformation
Momentum p_x	Translation $\mathrm{d}x$
Energy H	Time evolution: $\mathrm{d}t$
Angular momentum J_x	Rotation about x axis

1.2 From classical mechanics to commutators in quantum mechanics

This part is discussed in secion 3.1 of [1].

The commutation relationship is obtained by considering infinitesimal transformation. In general, classical rotation can be decomposed into rotation about three axes. We can use linear transformation to express them. For example, rotation about z axis is:

$$R_z(\phi) = \begin{pmatrix} \cos(\phi) & -\sin(\phi) & 0 \\ \sin(\phi) & \cos(\phi) & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{1.2.1}$$

Put it into infinitesimal amount, one has:

$$R_z(\varepsilon) = \begin{pmatrix} 1-\frac{\varepsilon^2}{2} & -\varepsilon & 0 \\ \varepsilon & 1-\frac{\varepsilon^2}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{1.2.2}$$

Similar procedure could be done for other axes (see equation 3.1.4 and 3.1.5 in [1]). By calculation one finds that

$$R_x(\varepsilon)R_y(\varepsilon) = R_y(\varepsilon)R_x(\varepsilon)$$

if terms higher than ε is ignored. This means that infinitesimal rotation $\mathrm{d}\omega$ can be safely considered as vectors.

However if only terms of order equal and lower than ε^2 is kept (note especially that ε^4 is ignored), one finds:

$$R_x(\varepsilon)R_y(\varepsilon) - R_y(\varepsilon)R_x(\varepsilon) = R_z(\varepsilon^2) - \mathbb{I} \tag{1.2.3}$$

Expand equation 1.1.8 in orders of ϕ and keep only terms with order $leq\phi^2$, we have:

$$\mathscr{D}(x,\varepsilon) = 1 - \frac{iJ_x\varepsilon}{\hbar} - \frac{J_x^2\varepsilon^2}{2\hbar^2}$$

and so on for other axes.

Plug these results into the classical commutation relationship 1.2.3, and with some calculation, one will find:

$$[J_i, J_j] = i\hbar\varepsilon_{ijk}J_k \tag{1.2.4}$$

here ε_{ijk} is the Levi-Civita notation in 3 dimension. This relation also ensures that the operator $\mathbf{J}$ we defined indeed corresponds to a physical rotation, which answers the question is mentioned in page 3.

1.3 From commutators to eigenvalues

Now one may use the commutation relation 1.2.4 to get the eigenvalues of these operators. The procedure is quite standard and can be found in section 3.5 of [1]. There the author defines the ladder operators:

Definition 1.1 (Ladder operator)**.**

$$J_\pm \equiv J_x \pm iJ_y \tag{1.3.1}$$

Then he derives the cummutation relationship:

$$[\mathbf{J}^2, J_k] = 0 \tag{1.3.2}$$
$$[J_+, J_-] = 2\hbar J_z \tag{1.3.3}$$
$$[J_z, J_\pm] = \pm\hbar J_\pm \tag{1.3.4}$$
$$[\mathbf{J}^2, J_\pm] = 0 \tag{1.3.5}$$
$$\tag{1.3.6}$$

Chossing the z direction as eigenstate. Denote the simultaneous eigenstates of $\mathbf{J}^2$ and J_z as $|j,m\rangle$, such that:

$$\mathbf{J}^2 |j,m\rangle = j(j+1)\hbar^2 |j,m\rangle \tag{1.3.7}$$
$$J_z |j,m\rangle = m\hbar |j,m\rangle \tag{1.3.8}$$

(such a strange choice is conventional in the case of spin).

As usual, one finds that

- For J_z, $J_\pm$ will pull up/lower its eigenvalue for eigenstate in units of $\hbar$.
- For $\mathbf{J}^2$, $J_\pm$ will not alter its eigenvectors, since it commutes with $\mathbf{J}^2$.

By above relationships, one can derive the following facts (for convenience let a be the eigenvalue for $\mathbf{J}^2$, and b be the eigenvalue for J_z.):

- $a \geq b^2$, i.e b is bounded by a. More specifically,
- $a = b_{\max}(b_{\max} + \hbar)$.
- Also, $-b_{\max} \leq b \leq b_{\max}$.
- Using $b_{\max} = b_{\min} + n\hbar$ (n is some integer), one gets
- $b_{\max} = \frac{n\hbar}{2}$. This, by identifying $j = \frac{n}{2}$, one has

$$a = j(j+1)\hbar^2 \tag{1.3.9}$$
$$b = m\hbar \tag{1.3.10}$$
$$(m = -j, -j+1, \cdots, j-1, j;\ j = \frac{n}{2})$$

1.4 Getting the matrix of rotation operators

Simply by commutation relationships above, one can easy get:

$$\langle j', m'|\, \mathbf{J}^2 \,|j, m\rangle = j(j+1)\hbar^2 \delta_{j'j}\delta_{m'm} \tag{1.4.1}$$
$$\langle j', m'|\, J_z \,|j, m\rangle = m\hbar\delta_{j'j}\delta_{m'm} \tag{1.4.2}$$
$$\langle j', m'|\, J_\pm \,|j, m\rangle = \sqrt{(j \mp m)(j \pm m + 1)}\hbar\delta_{j'j}\delta_{m',m\pm1} \tag{1.4.3}$$

To get matrix element for $\exp\left(\frac{-i\mathbf{J}\cdot\hat{\mathbf{n}}\phi}{\hbar}\right)$, one needs to use Euler angles.

1.4.1 Eulerian Angles

The Euler angles is discussed in section 3.3 of [1]. However, Sakurai's usage in his book [1] is a bit different from the usual one. But the following graph taken from that section should explains all:

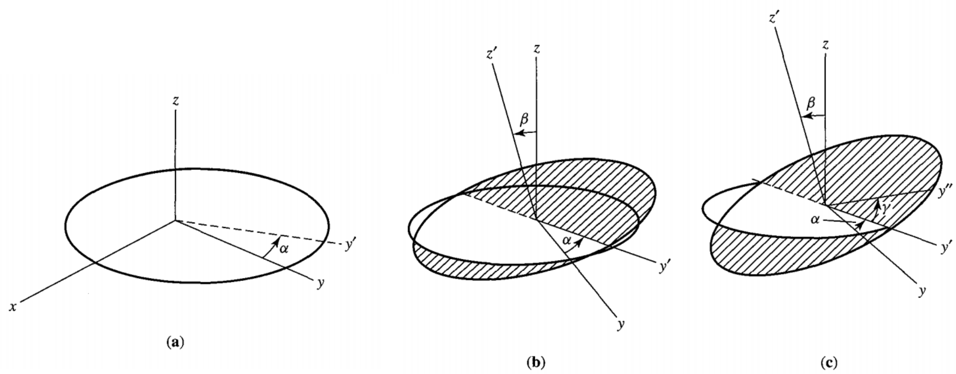

Figure 1: Euler Angles (fig 3.4 in that book)

One can find that a Euler rotaion characterized by (α, β, γ) could be decomposed into:

$$R(\alpha,\beta,\gamma) = R_z(\alpha)R_y(\beta)R_z(\gamma) \tag{1.4.4}$$

1.4.2 Using Euler angles to get matrix for rotation operator

As the title suggests, in section 3.5 of [1], we have

$$\exp\left(\frac{-i\mathbf{J}\cdot\hat{\mathbf{n}}\phi}{\hbar}\right) = \exp\left(\frac{-iJ_z\alpha}{\hbar}\right)\exp\left(\frac{-iJ_y\beta}{\hbar}\right)\exp\left(\frac{-iJ_z\gamma}{\hbar}\right)$$

, define

$$\mathscr{D}^{(j)}_{m'm} \equiv \langle j,m'|\exp\left(\frac{-iJ_z\alpha}{\hbar}\right)\exp\left(\frac{-iJ_y\beta}{\hbar}\right)\exp\left(\frac{-iJ_z\gamma}{\hbar}\right)|j,m\rangle \tag{1.4.5}$$

This $\mathscr{D}$ is sometimes called the **Wigner function**. Note that we have implicitly assumed that the rotation in $\exp\left(\frac{-i\mathbf{J}\cdot\hat{\mathbf{n}}\phi}{\hbar}\right)$ does not alter the eigenstate of length $\mathbf{J}^2$. This is physically satisfying, and can also be proved (equation 3.5.43 in [1]).

Since we have diagonalize using the eigenstate of J_z, we have:

$$\mathscr{D}^{(j)}_{m'm} = e^{-i(m'\alpha+m\gamma)}\langle j,m'|\exp\left(\frac{-iJ_y\beta}{\hbar}\right)|j,m\rangle \tag{1.4.6}$$

The remaining part can only be calculated case by case. Denote it as $d^{(j)}_{m'm}$, i.e.:

$$d^{(j)}_{m'm} \equiv \langle j,m'|\exp\left(\frac{-iJ_y\beta}{\hbar}\right)|j,m\rangle \tag{1.4.7}$$

Detailed calculation could start from equation 1.4.3. In case of $j=\frac{1}{2}$, as is familiar for use, it is:

$$d^{\frac{1}{2}} = \begin{pmatrix} \cos\left(\frac{\beta}{2}\right) & -\sin\left(\frac{\beta}{2}\right) \\ \sin\left(\frac{\beta}{2}\right) & \cos\left(\frac{\beta}{2}\right) \end{pmatrix} \tag{1.4.8}$$

Footnote [1]

1.4.3 Pauli matrices in half-spin: about $e^{-i\pi S_y/\hbar}$

Since everyone is familiar with the Pauli matrices in spin 1/2 system, I here only shows a useful result. This result is related to equation (4.4.65) in [1].

Since

$$S_y = \frac{\hbar}{2}\sigma_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

[1] This can also be obtained using the Pauli matrices, which can be found in my miscellaneous notes.

It is easy to check that $\sigma_y^2 = \mathbb{I}$. So:

$$\begin{aligned} e^{-i\phi S_y/\hbar} = e^{-i\frac{\phi}{2}\sigma_y} &= \sum_{n=0}^{\infty} \frac{(-i\frac{\phi}{2})^n(\sigma_y)^n}{n!} \\ &= \sum_{\text{odd } n} -\frac{i(\frac{\phi}{2})^n}{n!}\sigma_y + \sum_{\text{even } n} \frac{(i\frac{\phi}{2})^n}{n!}\mathbb{I} \end{aligned}$$

Using the taylor expansions:

$$\sinh x = \sum_{n=0}^{\infty} \frac{x^{2n+1}}{(2n+1)!} \text{ (odd terms)} \tag{1.4.9}$$

$$\cosh x = \sum_{n=0}^{\infty} \frac{x^{2n}}{(2n)!} \text{ (even terms)} \tag{1.4.10}$$

We see that:

$$e^{-i\phi S_y/\hbar} = e^{-i\frac{\phi}{2}\sigma_y} = -\sigma_y \sinh i\frac{\phi}{2} + \mathbb{I}\cosh i\frac{\phi}{2}$$

$$= -i\sigma_y \sin\frac{\phi}{2} + \mathbb{I}\cos\frac{\phi}{2} \tag{1.4.11}$$

$$= -i\frac{2}{\hbar}S_y \sin\frac{\phi}{2} + \mathbb{I}\cos\frac{\phi}{2} \tag{1.4.12}$$

$$= \begin{pmatrix} \cos(\frac{\phi}{2}) & -\sin(\frac{\phi}{2}) \\ \sin(\frac{\phi}{2}) & \cos(\frac{\phi}{2}) \end{pmatrix} \tag{1.4.13}$$

So

$$e^{-i\pi S_y/\hbar} = -i\frac{2S_y}{\hbar}$$

By exactly the same argument, or simply by the symmetry ($x \leftrightarrow y$), we have:

$$e^{-i\phi S_x/\hbar} = e^{-i\frac{\phi}{2}\sigma_x} = -i\sigma_x \sin\frac{\phi}{2} + \mathbb{I}\cos\frac{\phi}{2} \tag{1.4.14}$$

$$= -i\frac{2}{\hbar}S_x \sin\frac{\phi}{2} + \mathbb{I}\cos\frac{\phi}{2} \tag{1.4.15}$$

$$= \begin{pmatrix} \cos(\frac{\phi}{2}) & -\sin(\frac{\phi}{2}) \\ \sin(\frac{\phi}{2}) & \cos(\frac{\phi}{2}) \end{pmatrix} \tag{1.4.16}$$

Also, one can easily find that:

$$e^{-i\phi S_z/\hbar} = e^{-i\frac{\phi}{2}\sigma_z} = \begin{pmatrix} e^{-i\frac{\phi}{2}} & 0 \\ 0 & e^{i\frac{\phi}{2}} \end{pmatrix} \tag{1.4.17}$$

Also, we have a formula that encompass all the above relationship (proved in page 170, section 3.2 of [1]):

$$\exp\left(\frac{-i\vec{\sigma}\cdot\hat{\vec{n}}\phi}{2}\right) = \cos\left(\frac{\phi}{2}\right)\mathbb{I} - i\vec{\sigma}\cdot\hat{\vec{n}}\sin\left(\frac{\phi}{2}\right) \tag{1.4.18}$$

where $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$, and $\hat{\vec{n}}$ is any unit vector.

1.4.4 Eigenstate for $\mathbf{S} \cdot \hat{\mathbf{n}}$

Here is a physical arguemnt to construct an eigenstate for the operator $\mathbf{S} \cdot \hat{\mathbf{n}}$. It mimics what was done in page 172 of [1]. This is certainly correct when $j = \frac{1}{2}$. However, I am not sure about its validity in case of higher spin.

Suppose we have a state of the highest eigenvalue for J_z, i.e. a state labeled by $|j, j\rangle$, then in principle any state can be obtained from this state after a rotatation and a scale. But since $|\mathbf{n}\rangle$ is unit vector, it can be characterized by two angle: the polar angle β and the azimuthal angles α. As shown in the following picture:

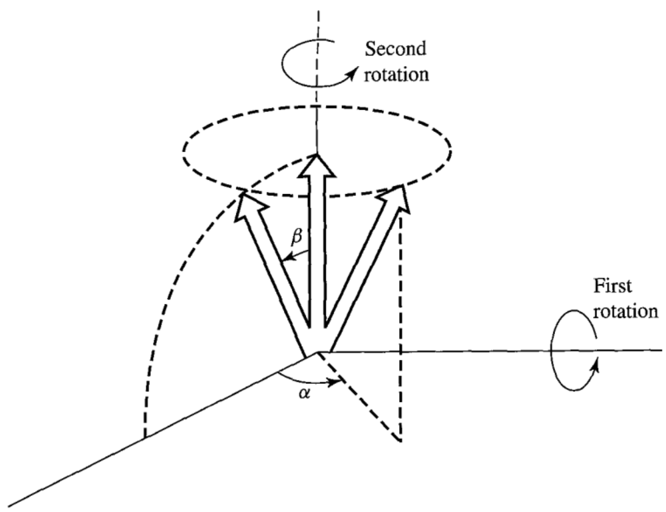

Figure 2: Polar and azimuthal angle (fig 3.3 in [1])

So I think the eigenstate should be:

$$|\hat{\mathbf{n}}; +\rangle = e^{-iS_z\alpha/\hbar} e^{-iS_y\beta/\hbar} |+\rangle \tag{1.4.19}$$

here $|+\rangle$ denotes the state $|j, j\rangle$. The eigenvalue is of course $j\hbar$.

This is confirmed when $j = \frac{1}{2}$ in page 171 of [1], but not in other cases.

2 Review of Symmetry Operator

This part is discussed in section 4.4 of [1].

Outline:

1. A note about antilinear operator, and we should treat it with care.
2. The invariance of probability and Wigner's theorem
3. The values of measurement before and after transformation

2.1 A note about antiunitary operator

Please note that the Dirac bra-ket notation is only convenient when we are dealing with unitary operators. When antiunitary operators, or arbitrary operators are considered, the situation can get tricky. Here are two examples.

2.1.1 Formula for base transformation

Suppose we transform the basis $|e_i\rangle$ by an operator $\mathcal{O}$, what is the formula for the corresponding basis for the dual space? The requirement of dual basis requires that:

$$\langle \widetilde{e}_i| = \langle \widetilde{e}_i| U^{-1}$$

But by the "dual-correspondance" in Dirac notation, we expect:

$$\langle \widetilde{e}_i| = \langle \widetilde{e}_i| U^{\dagger}$$

The two notion coincide only when U is unitary.

Similarly, consider the operator $|e_i\rangle \langle e_i|$, if we perform a scale of the basis $|e_i\rangle \to \lambda |e_i\rangle$, then how will the above operator transform? Is it

$$|\lambda e_i\rangle \langle \lambda e_i|$$

or is it:

$$|\lambda^{-1} e_i\rangle \langle \lambda e_i|$$

Of course, when the transformation is unitary, the two notion coincide, because $\lambda^* = \lambda^{-1}$ implies $\lambda = \lambda^{-1}$.

2.1.2 The adjoint of antilinear operator

labelsec:The-adjoint-of-antilinear-operator

If we were to define adjoint of an antilinear operator, we might run into troubles with traditional definition. For example, suppose A is antilinear, let us multiply it with $c\mathbb{1}$, where c is just some nonzero constant.

We have:

$$\langle \phi | cA\psi \rangle = c \langle \phi | A\psi \rangle \tag{2.1.1}$$

on the other hand:

$$\begin{aligned} \langle \phi | cA\psi \rangle = \langle cA\psi | \phi \rangle^* = \langle \psi | A^\dagger c^* \phi \rangle^* = (c \langle \psi | A^\dagger \phi \rangle)^* \\ = c^* \langle A\psi | \phi \rangle^* = c^* \langle \phi | A\psi \rangle \end{aligned} \tag{2.1.2}$$

A contracdiction. Then, it was proposed, in the first answer to this Math.SE post [3], that we define the adjoint operator differently for antilinear operator A:

$$\langle A^\dagger v | w \rangle = \langle v | Aw \rangle^* \tag{2.1.3}$$

Then the above discrepancy will not exist anymore (easily confirmed).

Here I also include the complete answer for reference:

I) First of all, one should never use the [Dirac bra-ket notation](http://en.wikipedia.org/wiki/Bra-ket_notation) (in its ultimate version where an operator acts to the right on kets and to the left on bras) to consider the definition of [adjointness](http://en.wikipedia.org/wiki/Adjoint_operator), since the notation was designed to make the adjointness property look like a mathematical triviality, which it is not. See also [this](http://physics.stackexchange.com/q/43069/2451) Phys.SE post.

II) OP's question(v1) about the existence of the adjoint of an [antilinear](http://en.wikipedia.org/wiki/Antilinear_map) operator is an interesting mathematical question, which is rarely treated in textbooks, because they usually start by assuming that operators are $\mathbb{C}$-linear.

III) Let us next recall the mathematical definition of the adjoint of a linear operator. Let there be a [Hilbert space](http://en.wikipedia.org/wiki/Hilbert_space) H over a [field](http://en.wikipedia.org/wiki/Field_%28mathematics%29) $\mathbb{F}$, which in principle could be either real or complex numbers, $\mathbb{F}=\mathbb{R}$ or $\mathbb{F}=\mathbb{C}$. Of course in quantum mechanics, $\mathbb{F}=\mathbb{C}$. In the complex case, we will use the standard physicist's convention that the [inner product/sequilinear form](http://en.wikipedia.org/wiki/Sesquilinear_form) $\langle\cdot|\cdot\rangle$ is conjugated $\mathbb{C}$-linear in the first entry, and $\mathbb{C}$-linear in the second entry.

Recall [Riesz' representation theorem](http://en.wikipedia.org/wiki/Riesz_representation_theorem): For each continuous $\mathbb{F}$-linear functional $f:H\to\mathbb{F}$ there exists a unique vector $u\in H$ such that

$$\mathrm{tag}\{1\} f(\cdot) ~=~ \langle u|\cdot\rangle.$$

Let $A:H\to H$ be a continuous[1] $\mathbb{F}$-linear operator. Let $v\in H$ be a vector. Consider the continuous $\mathbb{F}$-linear functional

$$\mathrm{tag}\{2\} f(\cdot) ~=~ \langle v|A(\cdot)\rangle.$$

The value $A^{\dagger}v\in H$ of the adjoint operator $A^{\dagger}$ at the vector $v\in H$ is by definition the unique vector $u\in H$, guaranteed by Riesz' representation theorem, such that

$$\mathrm{tag}\{3\} f(\cdot) ~=~ \langle u|\cdot\rangle.$$

In other words,

$$\mathrm{tag}\{4\} \langle A^{\dagger}v|w\rangle ~=~ \langle u|w\rangle ~=~ f(w)=\langle v|Aw\rangle.$$

It is straightforward to check that the adjoint operator $A^{\dagger}:H\to H$ defined this way becomes an $\mathbb{F}$-linear operator as well.

IV) Finally, let us return to OP's question and consider the definition of the adjoint of an antilinear operator. The definition will rely on the complex version of Riesz' representation theorem. Let H be given a complex Hilbert space, and let $A:H\to H$ be an antilinear continuous operator. In this case, the above equations (2) and (4) should be replaced with

$$\text{tag}\{2'\} f(\cdot) \;=\; \overline{\langle v|A(\cdot)\rangle},$$

and

$$\text{tag}\{4'\} \langle A^{\dagger} v|w\rangle \;=\; \langle u|w\rangle \;=\; f(w) = \overline{\langle v|Aw\rangle},$$

respectively. Note that f is a $\mathbb{C}$-linear functional.
It is straightforward to check that the adjoint operator $A^{\dagger}$: $H \to H$ defined this way becomes an antilinear operator as well.
–
[1]We will ignore subtleties with [discontinuous/unbounded operators](http://en.wikipedia.org/wiki/Unbounded_operator), domains, [selfadjoint extensions](http://en.wikipedia.org/wiki/Extensions_of_symmetric_operators), etc., in this answer.

2.1.3 Conclusion

For antilinear operators, we should always working with it acting on the kets. See page 289 in section 4.4 of [1].

2.2 Properties of a symmetry operator

Consider a symmetry operation acting on states such that:

$$|\alpha\rangle \to |\widetilde{\alpha}\rangle \;\; |\beta\rangle \to |\widetilde{\beta}\rangle \tag{2.2.1}$$

We require that the probability, the most important thing in quantum mechanics, is unchaged:

$$|\,\langle\widetilde{\beta}|\widetilde{\alpha}\rangle\,| = |\,\langle\beta|\alpha\rangle\,| \tag{2.2.2}$$

Wigner has proved that[2], all such symmetry transformations can be characterized either by an unitary or an antiunitary operator. Also, any antiunitary operator θ can be expressed as

$$\theta = UK \tag{2.2.3}$$

where U is unitary, and K is complex conjugation. Three facts about K:

- *"acts only on any coefficient that multiplies a ket (and stands on the right of K)."*
- K also does not act on the base ket, i.e. $K\,|e\rangle = |e\rangle$.
- K's action depends heavily the base ket. This is obvious from the above two points. Of course, this is not important when every physical state is only projective. However, I still doubt whether this will call additional problem. [3]

[2] Though it was only mentioned in page 289 of [1].
[3]Consider $K\,|e\rangle = |e\rangle$, but when $|e\rangle = i\,|e'\rangle$, then $K\,|e\rangle = -i\,|e'\rangle = -\,|e\rangle$.

2.3 States and Operators after transformation

Let U be an unitary operator and A be an antiunitary operator. Suppose we have $|\alpha\rangle$ and $|\beta\rangle$, and regard both to be transformed under U and A. Let:

$$|\alpha_u\rangle = U|\alpha\rangle\,,\ |\alpha_a\rangle = A|\alpha\rangle \tag{2.3.1}$$

$$|\beta_u\rangle = U|\beta\rangle\,,\ |\beta_a\rangle = A|\beta\rangle \tag{2.3.2}$$

Then by defintion of unitary and antiunitary, we have:

$$\langle\beta_u|\alpha_u\rangle = \langle\beta|\alpha\rangle \tag{2.3.3}$$

$$\langle\beta_a|\alpha_a\rangle^* = \langle\beta|\alpha\rangle \tag{2.3.4}$$

For any operator $\mathcal{O}$, we have, after transformation:

$$\mathcal{O}_u = U\mathcal{O}U^\dagger \tag{2.3.5}$$

$$\mathcal{O}_a = A\mathcal{O}^\dagger A^{-1} \tag{2.3.6}$$

The two equation are mean to expresses the following idea:

$$\langle\alpha|\,\mathcal{O}\,|\beta\rangle = \langle\widetilde{\alpha}|\mathcal{O}_u|\widetilde{\beta}\rangle \tag{2.3.7}$$

$$\langle\alpha|\,\mathcal{O}\,|\beta\rangle = \langle\widetilde{\beta}|\mathcal{O}_a|\widetilde{\alpha}\rangle \tag{2.3.8}$$

Proof may be found on page 292 of [1].

3 TR operator

Finally I can turn to the TR operator. But before the formal discussion of time reversal, I should first note that the name **time reversal** is actually a misnomer. As mentioned in page 284, section 4.4 in [1]:

> What we do in this section can be more appropriately characterized by the term **reversal of motion**. Indeed, that is the phrase used by E. Wigner, who formulated time reversal in a very fundamental paper written in 1932.

This section can be found in section 4.4 of [1].

Outline:

1. Deduce the property of TR symmetry operator from classical picture.
2. The problem of degenracy and how a breaking of TR symmetry lifts this degenracy.

3.1 From classical notion to properties of TR symmetry

To get the time reversal operator, we can first look at the following equality (let T dentoes the time reversal operator):

$$\left(1 - \frac{iH}{\hbar}\delta t\right)T|\alpha\rangle = T\left(1 - \frac{iH}{\hbar}(-\delta t)\right)|\alpha\rangle \tag{3.1.1}$$

This follows from the following notion: a time reversed state is equivalent to the original state at an earlier time. Recall that $\left(1 - \frac{iH}{\hbar}\delta t\right)$ produces an infinitesimal time translation.

From equality 3.1.1, one finds:

$$-iHT = TiH \tag{3.1.2}$$

One can show that T **must be antilinear**. Because if one assumes that T is linear, one will find that the energy spectrum for time reversal symmetric system will always has symmetric energy spectrum (i.e. with both and symmetric positive and negative energy), which is not true.

So we have:

- T is antiunitary.
- $TH = HT$ for a time reversal symmetric state.

Recall that $T = UK$, and K is highly dependent on the basis chosen. So U will depend on the basis too. To get T in a basis $|e_i\rangle$, obviously we only need to consider the result of $K|e_i\rangle$. This however, is hard to determine. However we can argue that in case when the basis has some classical connection, then by the Correspondance Principle we have, for example:

$$T\hat{p}T^{-1} = -\hat{p} \tag{3.1.3}$$
$$T\hat{x}T^{-1} = \hat{x} \tag{3.1.4}$$
$$T\mathbf{J}T^{-1} = -\mathbf{J} \tag{3.1.5}$$

with these one can easily find:

$$T|p\rangle = |-p\rangle \tag{3.1.6}$$
$$T|x\rangle = |x\rangle \tag{3.1.7}$$
$$[x_i, p_j]T|\rangle = i\hbar\delta_{ij}T|\rangle \tag{3.1.8}$$

where $|\rangle$ stands for any ket. Then clearly, T is just complex conjugation for wave function $\Psi(x)$. But T acts on $\Psi(p)$ will produces $\Psi^*(-p)$. The case for eigenstate of spin is a little complicated, which will be discussed in section 3.3.

3.2 Properties of TR operator

Following is a useful theorem, which is easy to proof (proof can be found on page 294 of [1]):

Theorem 3.1. *When Hamiltonian is invariant under time reversal and the energy eigenket is nondegenerate; then the corresponding energy eigenfunction is real (or, more generally, a real function times a phase factor independent of x)*

Therefore, a complex eigenfunction almost means a degenrate state, or the system is not invariant under time reversal.

The next theorem is about T^2. Classically, since there is only two directions in time, we expect $T^2 = 1$. But quantum states are rays, so there is the freedom of phase. Then $T^2 = \phi$ for some $|\phi|^2 = 1$. But better, we have:

Lemma 3.1. $T^2 = \pm\mathbb{1}$

Proof. Proof can be found on page 34 of [2]. But the proof is so clever that I want to include it here. First observe that $UU^\dagger = \mathbb{1}$, implies that $U^*U^T = \mathbb{1}$ by transposing both sides. Next one use the expression $T = UK$ to expand T^2, only to find that $U = \phi U^T$, this means that $\phi^2 = 1$. Hence $\phi = \pm 1$. □

We then have the useful fact:

Fact 3.1. *For any kets $|\alpha\rangle, |\beta\rangle$, we have*

$$\pm \langle\alpha|T\beta\rangle = \langle\beta|T\alpha\rangle \tag{3.2.1}$$

The sign is the same as in $T^2 = \pm 1$. Specifically, one has

$$\langle\alpha|T\alpha\rangle = 0 \tag{3.2.2}$$

when $T^2 = -\mathbb{1}$.

Proof. This is simple by using $\langle T\alpha|T\beta\rangle = \langle\beta|\alpha\rangle$, and replacing $|\alpha\rangle$ with $|T\alpha\rangle$. □

3.3 Time reversal operator in system with spin j

Using my guess 1.4.19:

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

and by similar argument in that section 1.4.4, we can argue that the state with opposite direction is

$$|\hat{\mathbf{n}};-\rangle = e^{-iS_z\alpha/\hbar}e^{-iS_y(\beta+\pi)/\hbar}|+\rangle \tag{3.3.1}$$

Again, I am using notation $|-\rangle$ to denotes $|j,-j\rangle$.

Since time reversal reverses the angular momentum, I expects:

$$T|\hat{\mathbf{n}};+\rangle = \eta|\hat{\mathbf{n}};-\rangle \tag{3.3.2}$$

where η is just some unnecessay factor.

With above relationship, one can easily see that:

$$T = \eta e^{-i\pi J_y/\hbar}K \tag{3.3.3}$$

The proof is trivial for $j = \frac{1}{2}$, but I cannot find a proof for other values of j.

It is also interesting to note that in general:

Theorem 3.2.

$$T^2 = -1 \text{ if } j \text{ is a half-integer} \tag{3.3.4}$$

$$T^2 = 1 \text{ if } j \text{ is an integer} \tag{3.3.5}$$

However, this can only be proved when $j = \frac{1}{2}$, in which case the proof is also straightforward if we use the formula mentioned in section 1.4.3.

However, if we imagine a spin j system as composed all just of electrons of spin $\frac{1}{2}$, then we have a strong argument that the above formula is true.

3.4 Kramer's theorem and the lifting of degeneracy

When one is concerned with the energy spectrum, one encounters the Kramer's theorem, which says:

Theorem 3.3 (Kramer's theorem)**.** *For a system with halt-integer j spin, the degree of degeneracy is at least two.*

Proof. Let $|n\rangle$ be an energy eigenstate. If the system is time reversal symmetric, i.e. $[H, T] = 0$, then $T|n\rangle$ is another energy eigenstate with the same energy. Supposing there is no degeneracy, then we have

$$|n\rangle = e^{i\eta}T|n\rangle$$

for some $\eta \in \mathbb{R}$. Apply T on both sides, then we have

$$\begin{aligned} e^{-i\eta}T^2|n\rangle &= \pm e^{-i\eta}|n\rangle \\ &= T|n\rangle = e^{i\eta}|n\rangle \end{aligned}$$

Clearly this is a contracdiction unless $T^2 = 1$, which is true only for interger spin system by equation 3.3.5 and 3.3.4. $\square$

Another way to show this is presented in page 37 of [2]. That method is too troublesome and basis dependent [4] to be shown here. But it shows an interesting fact that $T^2 = -1$, actually implies that U, its unitary component mentioned in section 2.2, is antisymmetric. This is obvious when one juxtapose the following two facts:

$$U(U^*)^T = \mathbb{1}$$

$$T^2 = UKUK = UU^* = -\mathbb{1}$$

By Kramer's theorem, one also says that for system with half-integer spin, one *lift the degenracy by breaking the time reversal symmetry of the system.*

3.4.1 Argument against Bernevig's result

An additional point by Bernevig is about the transition probability $\langle T\psi| H |\psi\rangle$ from a state to its time reversed state.

Here I first mention two points:

1. When $TH = HT$, and $T = UK$, one can deduce $UH^* = HU$, or $U^*H = H^*U^*$, i.e. $(U^*)_{mp}H_{pn} = (H^*)_{mp}(U^*)_{pn}$.
2. As mentioned before in section 3.4, U is antisymmetric, so U^* is antisymmetric too.

[4] Borrowing the jargon of mathematicians, not canonical, geometric, or intrinsic.

Then begin Bernevig's wrong calculation (Summation implied when index is repeated twice):

$$\begin{aligned}
\langle T\psi|H|\psi\rangle &= (U_{mp}K\psi_p)^* H_{mn}\psi_n \\
&= U^*_{mp}\psi_p H_{mn}\psi_n \\
&= (U^\dagger)_{pm}\psi_p H_{mn}\psi_n \qquad (3.4.1)\\
&= (U^\dagger)_{pm}\psi_p (THT^{-1})_{mn}\psi_n \\
&= (U^\dagger)_{pm}\psi_p \left(U_{mr}KH_{rq}(-U_{qn}K)\right)\psi_n \\
&= -(U^\dagger)_{pm}\psi_p \left(U_{mr}H^*_{rq}U^*_{qn}\right)\psi_n \\
&= -\psi_p \left((U^\dagger)_{pm}U_{mr}\right) H^*_{rq}U^*_{qn}\psi_n \\
&= -\psi_p H^*_{pq}U^*_{qn}\psi_n \\
\text{(by point 1)} &= -\psi_p U^*_{pq}H_{qn}\psi_n \\
\text{(by point 2)} &= U^*_{qp}\psi_p H_{qn}\psi_n \\
\text{(by the first line)} &= \langle T\psi|H|\psi\rangle \qquad (3.4.2)
\end{aligned}$$

So I see that he just circles back to the origin...

No I give an argument that statement in page 37 of [2] cannot be true.

Argument 3.1. Suppose we can prove that $\langle T\psi|H|\psi\rangle = 0$. Then $\langle \psi|HT|\psi\rangle = 0$, notice that $H = THT^{-1}$, and $T^2 = -1$, one can see that $\langle\psi|H|\psi\rangle = 0$. Such is too strong an result. For example, if $|\psi\rangle$ is any eigenket of H, then our argument shows that its eigenvalue is zero. Does this means that H is just the trivial operator 0? Of course not! Therefore the Bernevig's result is wrong.

3.5 Time reversal symmetry in crystal

3.5.1 Time reversal symmetry in spinless crystal

Since there is not spin, time reversal symmetry does not alter a creation/annihilation of a particle. Then:

$$Tc_jT^{-1} = c_j \qquad (3.5.1)$$

Then, in the fourier expansion of c_j:

$$c_j = \sum_k e^{ikR_j} c_k \qquad (3.5.2)$$

Since T acting on the left, will change e^{ikR_j} into e^{-ikR_j}, then naturally:

$$Tc_kT^{-1} = c_{-k} \qquad (3.5.3)$$

Then, for a time reversal symmetric system, let $H = \sum_k h(k)c_k^\dagger c_k$. Since $THT^{-1} = H$, T has to flip the sign of k again, so:

$$Th(k)T^{-1} = h(-k) \text{ (For TR symmetric state)} \qquad (3.5.4)$$

Remark 3.1 (Implications for crystal systems)**.** *By equation 3.5.4, one has $\phi(k)$ and $T\phi(k)$ corresponding to two eigenstate in k and $-k$. But since $\langle\alpha|\,|T\alpha\rangle$ is not necessarily 0 for $T^2 = \mathbb{1}$, We cannot prove that we have a double generacy because the two candidate $h(k)$ and $h(-k)$ might be the same wave function.*

Another important implication is that

Theorem 3.4. *Hall Conductance vanishes for Spinless time symmetric system.*

Proof. Recall we have:

$$\sigma_{ij} = \int \frac{\mathrm{d}k_x\,\mathrm{d}k_y}{(2\pi)^2} \sum_{a=1}^{m} (-i) F^a_{jk}(\mathbf{k}) = \frac{1}{(2\pi)^2} \sum_{a=1}^{m} \gamma_a \tag{3.5.5}$$

i.e., The Hall conductivity is an integral over the filled bands of the Berry curvature. (See (3.79) of [2])

Here

$$F_{ij}(\mathbf{k}) = -i\left(\langle \partial_i u(k)|\partial_j u(k)\rangle - (i \leftrightarrow j)\right)$$

is the Berry field strength. For system with TR symmetry, we have

$$u(k) = Tu(-k)$$

(Note that T flips the sign of k) Since T is antiunitary, we have $u(-k) = u(k)^*$. Therefore $\langle \partial_i u(-k)|\partial_j u(-k)\rangle = \langle \partial_j u(k)|\partial_i u(k)\rangle$ So:

$$F_{ij}(-\mathbf{k}) = -F_{ij}(\mathbf{k}) \tag{3.5.6}$$

Therefore F_{ij} is a odd function. So its integration over the whole BZ is zero, i.e. σ_{ij} is zero. □

3.5.2 Time reversal symmetry in electron bands

Natually operator T flips the sign of the creation/annihilation operator of an electron. We now proves:

Theorem 3.5. *We have, up to a phase,*

$$Tc_\sigma T^{-1} = i(\sigma_y)_{\sigma\sigma'} c_{\sigma'} \tag{3.5.7}$$

$$Tc^\dagger_\sigma T^{-1} = ic^\dagger_{\sigma'} (\sigma_y)^T_{\sigma'\sigma} \tag{3.5.8}$$

Where $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$. *and σ label spin ↑ and spin ↓.*

Proof. Assuming

$$Tc_\uparrow T^{-1} = Ac_\downarrow \tag{3.5.9}$$

$$Tc_\downarrow T^{-1} = Bc_\uparrow \tag{3.5.10}$$

Then we need only to prove $AB^* = -1$. Since up to a phase change, we can let

$$A = 1\,, B = -1 \tag{3.5.11}$$

This is what the theorem says.

Let's consider the following

$$Tc_\uparrow c_\uparrow^\dagger |0\rangle$$

First, it is equal to $T|0\rangle$. On the other hand, we can let the T jumps over one creation operator:

$$Ac_\downarrow Tc_\uparrow^\dagger |0\rangle$$

Now insert $T^{-1}T$ between A and $c_\downarrow$. And makes the new T one jump to the right:

$$AT^{-1}Bc_\uparrow T^2 c_\uparrow^\dagger |0\rangle$$

Now be careful to notice that the first T^{-1} is T, whereas the second T^2 is $-\mathbb{1}$ (watch the Spin!). With simple calculation one finds it is equal to

$$-AB^*T|0\rangle$$

Hence $-AB^* = 1$. The case for the creation operatros is similar. □

Theorem 3.6. *For the creation and annihilation in the momentum space, we have:*

$$Tc_{\mathbf{k}\sigma}^\dagger T^{-1} = c_{-\mathbf{k}\sigma'}^\dagger i(\sigma_y)_{\sigma\sigma'}^T \tag{3.5.12}$$

$$Tc_{\mathbf{k}\sigma} T^{-1} = c_{-\mathbf{k}\sigma'} i(\sigma_y)_{\sigma\sigma'} \tag{3.5.13}$$

Proof. This is quite obvious since T changes the coefficient of fourier expansion: $e^{-i\mathbf{k}\cdot\mathbf{R}_j} \to e^{i\mathbf{k}\cdot\mathbf{R}_j}$ □

Then directly apply T and T^{-1} to both sides of

$$H = \sum_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger h^{\sigma\sigma'}(\mathbf{k}) c_{\mathbf{k}\sigma'}$$

gives (noticing $h(k)$ is just a number that T turns it into its conjugate number):

$$h^{\sigma\sigma'}(\mathbf{k}) \mapsto i(\sigma_y)_{\sigma_1\sigma}^T (h^{\sigma,\sigma'})^* i(\sigma_y)_{\sigma'\sigma_2} \tag{3.5.14}$$

If one carefully examine the cases, one finds that when $\sigma_1 \neq \sigma_2$, the above should obviously be 0. And when $\sigma_1 = \sigma_2$, the RHS above is surprisingly just $(h^{\{\cdot,\cdot\}})^*$, with appropriate spin. So we have compactly:

Theorem 3.7. *For electron bands,*

$$Th(\mathbf{k})T^{-1} = h(-\mathbf{k}) \tag{3.5.15}$$

with spin inverted.

Then we have the following fact:

Fact 3.2. *For Time reversal symmetric electron bands, there is always at least two degenerate state*

This is obvious since:

$$h(-\mathbf{k})T|u(\mathbf{k})\rangle = Th(\mathbf{k})|u(\mathbf{k})\rangle = TE(\mathbf{k})|u(\mathbf{k})\rangle = E(\mathbf{k})T|u(\mathbf{k})\rangle$$

Also, by fact 3.1, one sees that the time reversed state $T|u(\mathbf{k})\rangle$ is distinct from the orginal state. Hence the double degeneracy.

4 Anchor

References

[1] Modern Quantum Mechanics. J.J. Sakurai.

[2] Introduction to Topological Insulators. Bernevig.

[3] Existence of adjoint of an antilinear operator, time reversal

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