12 Time Reversal Symmetry in Quantum Mechanics

In classical mechanics, time reversal has the following effect on physical quantities:

$$t(\text{time}) \to -t, x(\text{position}) \to x, p(\text{momentum}) \to -p, E(\text{electric field}) \to E, B(\text{magnetic field}) \to -B \tag{1}$$

In quantum mechanics, we would expect similar relations to hold under time reversal. However, there is a problem. Consider the canonical commutation relation between position and momentum

$$[x, p] = i\hbar \tag{2}$$

If $x \to x$, $p \to -p$ under time reversal, then this commutation relation no longer holds.

How to solve this problem?

It was realized by Wigner that in quantum mechanics, time reversal has to be defined in a very special way different from all other symmetries. Time reversal operator is anti-unitary: it maps i to $-i$. If this is the case, then the canonical commutation relation between x and p will remain invariant under time reversal.

The action of time reversal on a wave function then contains two parts: first take complex conjugation in a certain basis, then apply a linear transformation in this basis. That is, we can write

$$\mathcal{T} = UK \tag{3}$$

where K denotes complex conjugation and U denotes some unitary transformation.

Then time reversal acts on operators as

$$\mathcal{T}O\mathcal{T}^{-1} = UKOKU^\dagger = UO^*U^\dagger \tag{4}$$

That is, the action of time reversal on operators contains two parts: first take complex conjugation of the operator written in certain basis, then conjugate the operator by some unitary transformaiton in this basis.

Let's see what this anti-unitary property of time reversal implies.

0. Time reversal does not commute with complex numbers.

$$\mathcal{T}c\mathcal{T}^{-1} = c^* \tag{5}$$

1. Time reversal is not a linear operator on wave functions.

$$\mathcal{T}\left(\alpha_1\psi_1 + \alpha_2\psi_2\right) = \alpha_1^*\mathcal{T}(\psi_1) + \alpha_2^*\mathcal{T}(\psi_2) \tag{6}$$

Instead it is said to be anti-linear.

Are anti-linear operators allowed as symmetry operators in quantum mechanics? The answer is yes, because:

2. Under time reversal, the absolute value of wave function inner product remains invariant.

To see this, notice that

$$\mathcal{T}\psi_1 = U\psi_1^*, \mathcal{T}\psi_2 = U\psi_2^* \tag{7}$$

Therefore,

$$\langle \mathcal{T}\psi_1 | \mathcal{T}\psi_2 \rangle = \langle \psi_1^* | U^\dagger U | \psi_2^* \rangle = \langle \psi_1 | \psi_2 \rangle^* \tag{8}$$

The inner product between any two wave functions does not remain invariant, but that is not a problem because the absolute value of the inner product is and only the absolute value is experimentally measurable. In fact, Wigner showed that in order for the absolute value of inner product be invariant, the symmetry operation must either be unitary or anti-unitary.

3. Representations of time reversal symmetry.

Time reversal, as its name suggests, forms a C_2 symmetry group, $\mathcal{T}^2 = 1$. However, the representations of time reversal symmetry are very different from that of usual C_2 symmetry groups, which have unitary representations.

Let's first look for one dimensional representations of time reversal symmetry. That is, we are looking for quantum states which transform under time reversal as

$$\mathcal{T}|\psi\rangle = e^{i\theta}|\psi\rangle \tag{9}$$

Applying time reversal again, we get

$$\mathcal{T}^2|\psi\rangle = e^{-i\theta}\left(\mathcal{T}|\psi\rangle\right) = e^{-i\theta}e^{i\theta}|\psi\rangle = |\psi\rangle \tag{10}$$

Therefore, the 'quantum number' of time reversal symmetry $e^{i\theta}$ can be any complex number of absolute value 1. It may seem that time reversal has an infinite number of one dimensional representations, but in fact they are all equivalent to each other. If we apply a basis transformation $|\psi'\rangle = e^{i\alpha}|\psi\rangle$, then

$$\mathcal{T}|\psi'\rangle = e^{-i\alpha}e^{i\theta}|\psi\rangle = e^{-i2\alpha}e^{i\theta}|\psi'\rangle \tag{11}$$

By tuning α, we can change from one θ to any other θ'. Therefore, in this sense, time reversal has only one (trivial) one dimensional representation. In fact, this is the only linear representation of time reversal.

On the other hand, time reversal has an interesting projective representation. Consider the action of

$$\mathcal{T} = 2i\sigma_y K = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} K \tag{12}$$

on the Hilbert space of a spin 1/2. $\mathcal{T}$ applies the expected operation to all spin operators

$$\mathcal{T}\sigma_x\mathcal{T}^{-1} = -\sigma_x, \mathcal{T}\sigma_y\mathcal{T}^{-1} = -\sigma_y, \mathcal{T}\sigma_z\mathcal{T}^{-1} = -\sigma_z \tag{13}$$

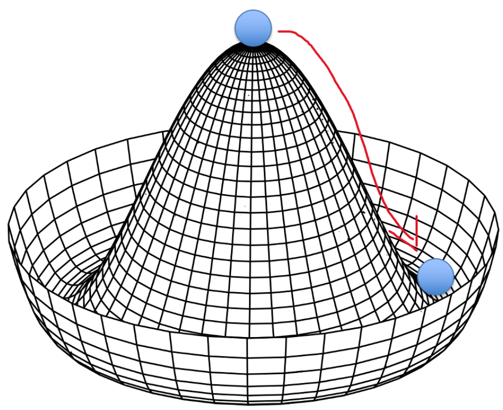
That is, it reverses the direction of spin – a magnetic dipole moment. However, this representation is not linear

$$\mathcal{T}^2 = -1 \tag{14}$$

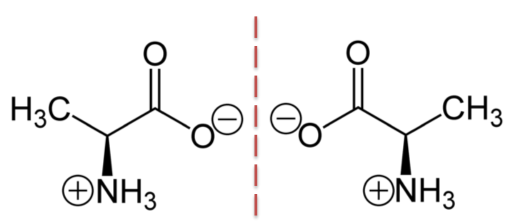
It is a projective representation of time reversal and more interestingly it has to be at least two dimension (can you show it?). As fermions all have spin 1/2, we say that fermions transform under time reversal as $\mathcal{T}^2 = -1$.

13 Spontaneous Symmetry Breaking

Even when a physical system has certain symmetry, the lowest energy state may spontaneously break that symmetry. This has a lot of implication for the low energy excitations in the system. The simplest illustration of this idea is the Mexican hat. The shape of the hat (hence the potential energy) is invariant under the rotation around the vertical axis. If we put a ball at the top of the hat, that is an unstable equilibrium point and under small perturbation the ball would go downhill (downhat) into the valley. Each point in the valley has the lowest potential energy so is a stable equilibrium point. The ball may roll into any of these points but once it does, the rotation symmetry of the system is broken. Exactly which point the ball rolls into depends on the details of the initial perturbation.



Another example is the chiral molecule. Chiral molecules are ones that break mirror reflection symmetry. In 3D space, if we choose the mirror plane to be the xz plane, then mirror reflection operates as $x \to x, y \to -y, z \to z$. It generates a Z_2 group. Chiral molecules are not invariant under such transformations, although the equation of motion – the Schrodinger's equation for the nucleus and electrons – is invariant. Therefore, the wave-function of a chiral molecule does not form a 1D representation of the Z_2 group. Instead, the 'left-handed' molecule and the 'right-handed' molecule map into each other under the symmetry transformation and together form a two dimensional reducible representation of the symmetry and the two configurations have the same energy. The fact that chiral molecules break mirror reflection symmetry means that they can interact with light in a different way. Suppose that we shine a light linearly polarized in the z direction onto the molecule. The electric field in the light points in the z direction and is hence invariant under mirror reflection. If the molecule is reflection symmetric, then the light coming out of the molecule would also be reflection symmetric. On the other hand, if the molecule is chiral, the outgoing light may also be chiral. That is, the outgoing light may be circularly polarized, described by a light vector $z + iy$. Under mirror reflection, the light vector becomes $z - iy$.



The prototypical spontaneous symmetry breaking in a many-body system is a magnet. Consider a system of classical magnetic moments. Let's start in 1D and consider the case where the magnetic moments are constrained to point either in the positive or negative z direction with the moment being $S_z = \pm 1$. The magnetic moments interact with their neighbors: each pair has higher energy if their moments are opposite to each other and has lower energy if their moments point in the same direction.

$$E = -\sum_i S_i S_{i+1} \tag{15}$$

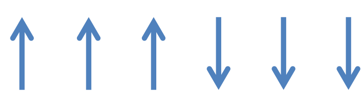
There are then two lowest energy states, one with all the moments pointing up and one with all the moments pointing down.

Now let's talk about symmetry. The system has a Z_2 symmetry of flipping magnetic moments. That is, the energy of the system remains invariant if we flip all the moments at the same time

$$S_i \to -S_i \tag{16}$$

However, each of the lowest energy states break this symmetry. Under the symmetry transformation, they map into each other and they always have the same energy.

Low energy excitations then exist in the form of a domain wall between the two states. That is, we can have the left hand side of the system in the up state and the right hand side of the system in the down state. Within each half system, the energy of the system is minimized, but interface between them has a finite energy cost of 2. In a system with periodic boundary condition, there are always an even number of domain walls. If we create a pair of domain walls, let them propagate through the system and re-annihilate with each other, we can flip the up domain into the domain domain and vice verse.



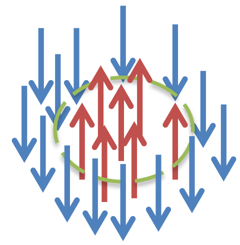
In two dimensions, we can have a similar model with moments restricted to the z direction and interaction energy being

$$E = -\sum_i S_i S_{i+1} \tag{17}$$

Again the system has the Z_2 symmetry of flipping moments and the two lowest energy states break this symmetry. The difference from the 1D case is that the domain wall between two domains now takes the form of a loop. Magnetic moments on the two sides of the loop are opposite to each other and the energy cost of the domain wall grows with its length. Therefore, if we want to flip one lowest energy state into the other by creating a domain wall and letting it sweep across the whole system, the energy barrier in the whole process is proportional to the linear size of the system. Compare to the care of 1D where the energy cost of flipping domains is only finite.

Now back to 1D and let's consider the more interesting case where the moments are constrained to the xy plane. $\vec{S}_i$ is now a vector and can point in any direction in the two dimensional plane. The interaction between the moments still prefer to have them aligned and the total energy is given by

$$E = -\sum_i \vec{S}_i \cdot \vec{S}_{i+1} \tag{18}$$



The system has a $U(1)$ symmetry of (global) rotation around the z axis while the lowest energy state breaks this symmetry. In the lowest energy state, the moments all point in the same direction. The direction can be arbitrary (within the 2D plane) and different lowest energy states are mapped into each other under the global rotation symmetry.

The low energy excitation of the system now comes in the form of a spin wave. Suppose that we start from a lowest energy state. Instead of doing global rotation, we can apply small rotations in a space time dependent way. If we choose the rotation angle to be

$$\theta(i) = \theta_0 \cos(k \cdot i) \tag{19}$$

then each nearest neighbor pair of moments are slightly mis-aligned, giving rise to a total energy of

$$E = -|S|^2 \sum_i \cos(\theta_{i+1} - \theta_i) \approx -|S|^2[-N + \theta_0^2 \sum_i (\cos(k \cdot i + 1) - \cos(k \cdot i))^2] \tag{20}$$

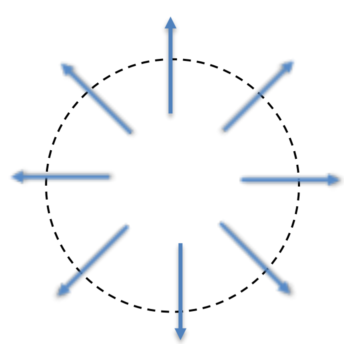
where the approximation depends on the fact that θ_0 is small. In the long wavelength limit where

$k << 1$, we can see that the energy difference between such spin wave states and the lowest energy states scales as k^2. That is, the excitation energy goes to zero in the long wavelength limit and the spin wave has a quadratic dispersion.

A more interesting type of low energy excitation is a topological one. Suppose that in a 1D system with periodic boundary condition, starting from the lowest energy state, we rotate the moments with angle

$$\theta_n = \frac{2\pi n}{N} \tag{21}$$

where N is the total number of moments. If we trace the direction of the moments around the



ring, we see that they rotate by 2π. This is called the winding number of the moments. It can only take values of integer multiples of 2π which is a discrete set of numbers. This configuration is fundamentally different from the spin wave one in that it cannot be smoothly deformed back to the lowest energy state. If we smoothly deform a state, we cannot change its winding number. This excitations is said to be topological and costs energy

$$\Delta E \sim \frac{1}{N} \tag{22}$$