PHYS-505

Parity and other Discrete Symmetries

Lecture-7

Discrete Symmetries

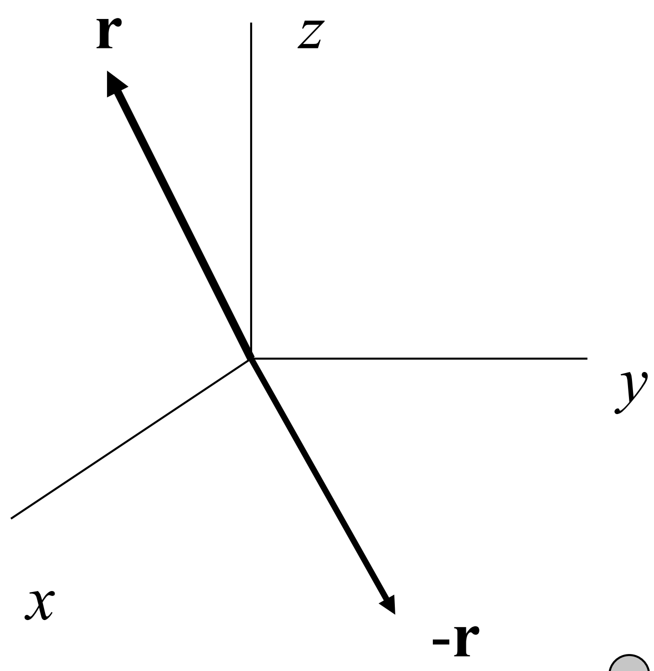
- So far we have considered continuous symmetry operators – that is, operations that can be obtained by applying successively infinitesimal symmetry operations. Not all symmetry operations useful in quantum mechanics are necessarily of this for. Parity, lattice translation and time reversal are examples of these.

Space Reversal Symmetry and the Concept of Conservation

- Consider now a case where the potential is constant under space reversal i.e $V(\mathbf{r}) = V(-\mathbf{r})$, or in a mathematical language the potential is an even function of $\mathbf{r}$.
- In the above case the Hamiltonian has a **space reversal symmetry**. As we have seen symmetries are always connected to conservations laws. Is there any conserved quantity which corresponds to the space reversal symmetry?
- The answer is yes and this quantity is called the **parity.**

Parity and Space Reversal

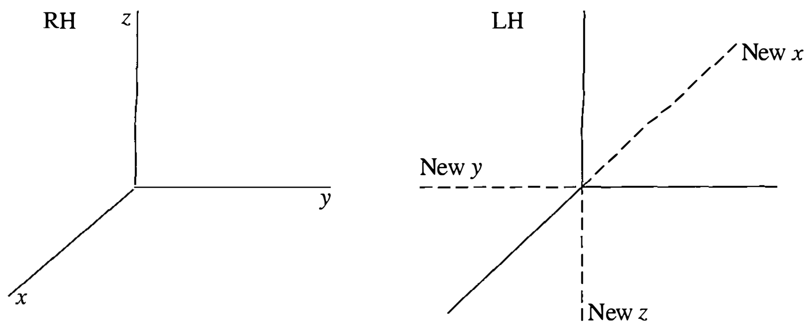
- In quantum mechanics there is another physical quantity which is conserved while it does not have a classical counterpart. This quantity is **parity**.
- **Definition:** We call space reversal (or inversion) the geometric action **r** --> -**r** which maps every space point at is diametric with respect to the origin of the coordinate system.



It is more convenient than a simple reflection because you need specify only the point which is at the center of symmetry.

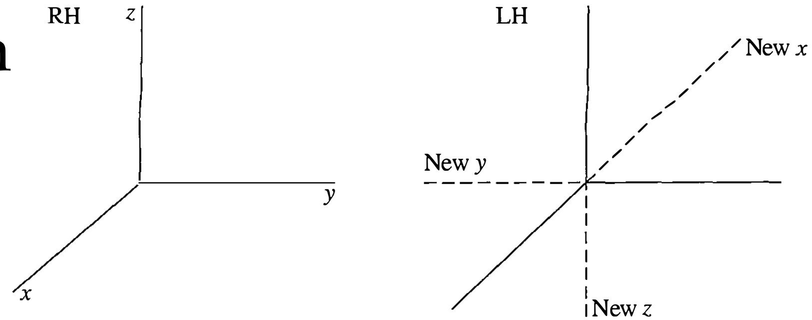
Parity and Space Reversal

- The space reversal is equivalent to a change of a right-handed (RH) system into a left-handed system (LH) system as shown in figure.
- Let's focus on transformation of kets and not system of axis. We introduce the parity operator **P**.



Parity and Space Reversal

- The basic requirement is the expectation value of a **r** taken with respect to the inverted state to be opposite in sign:



$$\langle a|\mathbf{P}^{+}\mathbf{r}\mathbf{P}|a\rangle = -\langle a|\mathbf{r}|a\rangle$$

- This is accomplished if

$$\mathbf{P}^{+}\mathbf{r}\mathbf{P} = -\mathbf{r} \Rightarrow \{\mathbf{P},\mathbf{r}\} = 0$$

Anti-commutation

Parity and Space Reversal

- The parity operator *P* is a hermitian operator which has the following properties:

$$\mathbf{P}\psi(\mathbf{r}) = \psi(-\mathbf{r}) \qquad\qquad \mathbf{P}^2 = \mathbf{P}\cdot\mathbf{P} = \mathbf{1}$$

- The eigenvalues of this operator can be shown to be +1, -1. The eigenfunctions which correspond to the positive value +1 are even functions (or functions with *positive parity*), while the eigenfunctions which correspond to the negative value -1 are odd functions (or functions with *negative parity*).

Parity and Symmetry

- Classically, if a state is symmetric under an inversion, the operation gives back the same state. In quantum mechanics, however, there are the two possibilities: we get the *same state* or *minus* the same state. When we get the *same* state, we say that the state has *even parity*. When the sign is reversed we say that the state has *odd parity*.
- There are, of course, states which are not symmetric under the operation **P**; these are states with no definite parity. For instance, in the H_2^+ system the state $|\mathrm{I}\rangle = (|1\rangle + |2\rangle)/\sqrt{2}$ has even parity, the state $|\mathrm{I}\rangle = (|1\rangle - |2\rangle)/\sqrt{2}$ has odd parity, and the state $|\mathrm{I}\rangle = |1\rangle$ has no definite parity.

Parity and Symmetry

- Many of the *laws* of physics—but not all—are unchanged by a reflection or an inversion of the coordinates. They are *symmetric* with respect to an inversion. The laws of electrodynamics, for instance, are unchanged if we change x to $-x$, y to $-y$, and z to $-z$ in *all* the equations. The same is true for the laws of gravity, and for the strong interactions of nuclear physics.

Parity and Symmetry

- Only the weak interactions—responsible for β-decay —do not have this symmetry. We will for now leave out any consideration of the β-decays. Then in any physical system where β-decays are not expected to produce any appreciable effect—an example would be the emission of light by an atom—the Hamiltonian **H** and the operator **P** will commute.

Parity and Symmetry

- Under these circumstances we have the following proposition. If a state originally has even parity, and if you look at the physical situation at some later time, it will again have even parity. For instance, suppose an atom about to emit a photon is in a state known to have even parity. You look at the whole thing—including the photon—after the emission; it will again have even parity (likewise if you start with odd parity). This principle is called the *conservation of parity*.

Parity and Symmetry

- You can see why the words "conservation of parity" and "reflection symmetry" are closely intertwined in the quantum mechanics. Although until a few years ago it was thought that nature always conserved parity, it is now known that this is *not* true. It has been discovered to be false because the β-decay reaction does not have the inversion symmetry which is found in the other laws of physics.

Parity and Symmetry

- Now we can prove an interesting theorem (which is true so long as we can disregard weak interactions):
- **"Any state of definite energy which is not degenerate must have a definite parity. It must have either even parity or odd parity".**
- Remember that we have sometimes seen systems in which several states have the same energy—we say that such states are *degenerate*. Our theorem will not apply to them.

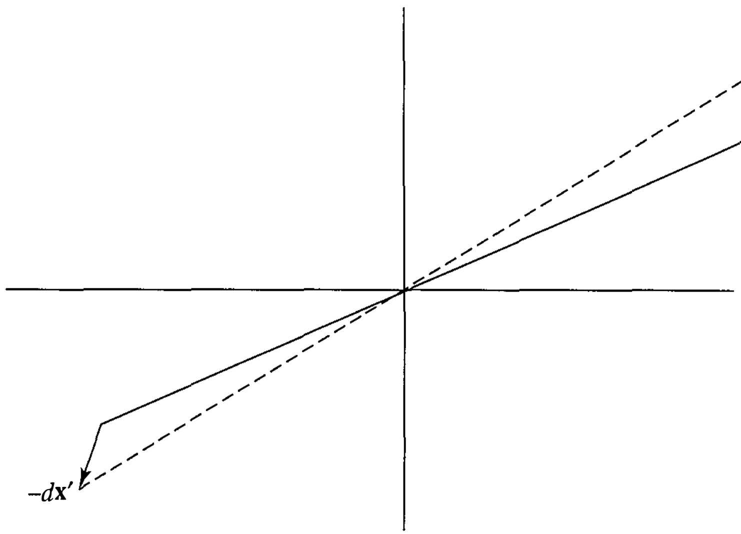
Parity and other Vectors

- The parity operator **P** has the following effect on the momentum operator:

$$\{\mathbf{P},\mathbf{p}\}=0 \Rightarrow \mathbf{P}^{+}\mathbf{p}\mathbf{P}=-\mathbf{p}$$

- The parity operator **P** has the following effect on the angular momentum operator:

$$[\mathbf{P},\mathbf{J}]=0 \Rightarrow \mathbf{P}^{+}\mathbf{J}\mathbf{P}=\mathbf{J}$$



Translation followed by parity and vice versa

Parity and other Vectors

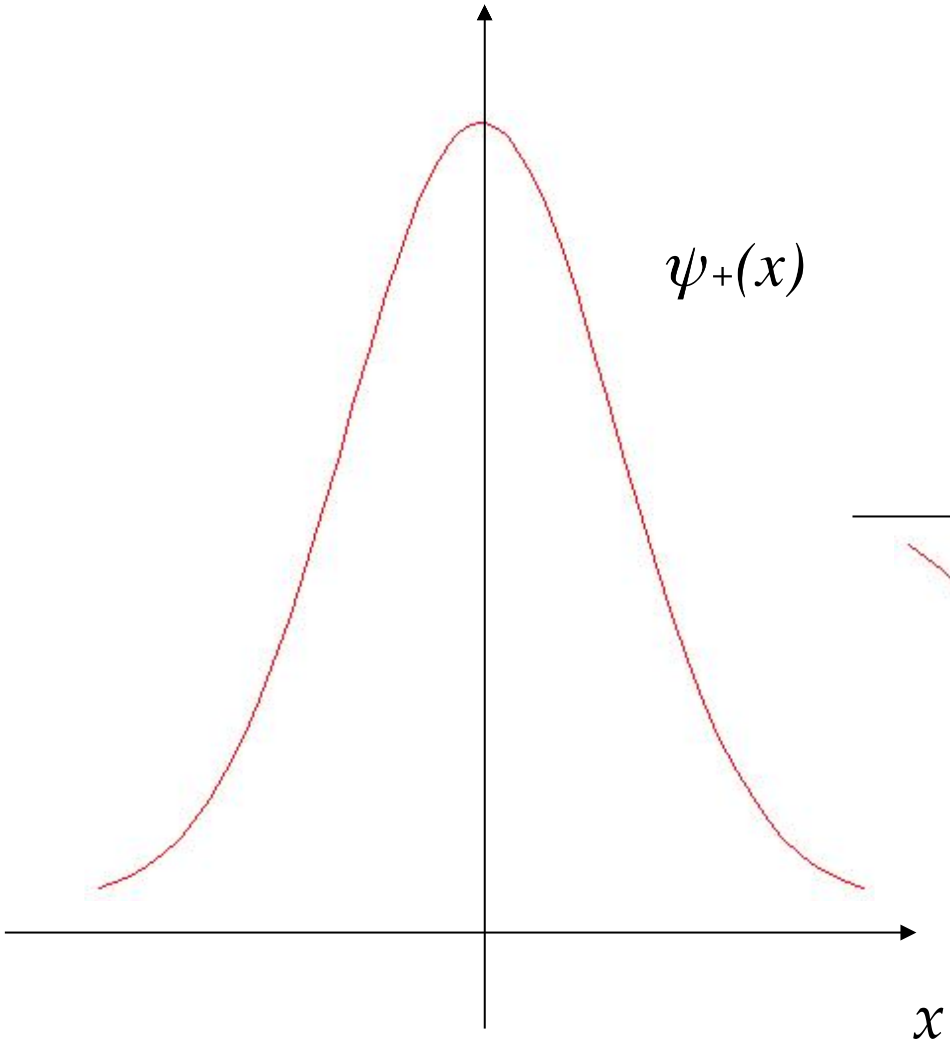
- Under rotations, **r** and **J** transform in the same way, so they are both vectors, or spherical tensors of rank 1.
- However **r** (or **p**) is odd under parity, whereas **J** is even under parity. Vectors that are odd under parity are called **polar vectors**, and vectors that are even under parity are called **axial vectors**, or **pseudovectors**.

Parity and other Vectors

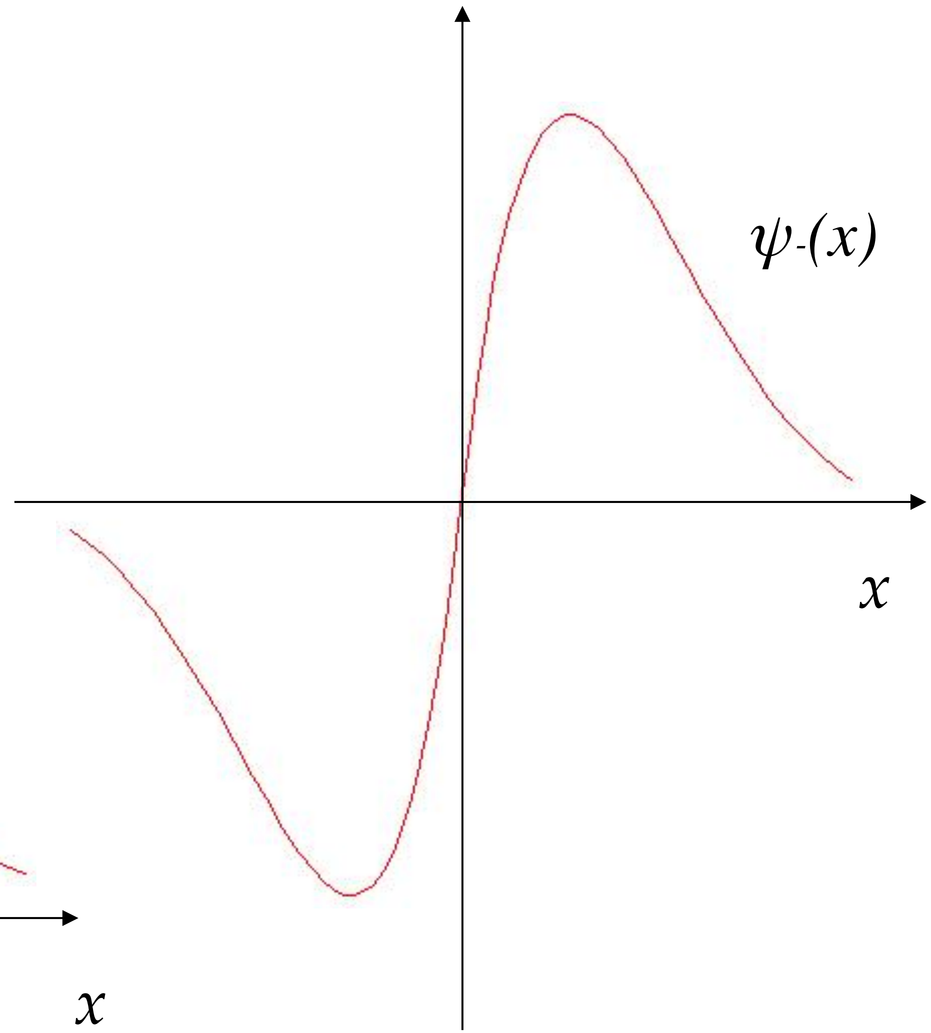
- For the wavefunction of a spinless particle we have the following relation:

$$\psi\left(-\mathbf{r}'\right) = \pm\psi\left(\mathbf{r}'\right)\begin{cases} \text{even parity} \\ \text{odd parity} \end{cases}$$

- Not all wavefunctions of physical interest have definite parities as above. Consider, for instance, the momentum eigenket. The momentum operator anticommutes with the parity operator, so the momentum eigenket is not expected to be parity eigenket. (E.g. a plane wave)



Even function
(parity +1)



Odd function
(parity -1)

Parity

- **Conclusion a**: If a system has space reversal symmetry, then parity is a conserved quantity.
- **Conclusion b**: If the wavefunction of a physical system, which has space reversal symmetry, is at a given instant even or odd, then it will remain even or odd respectively

Parity and Selection Rules

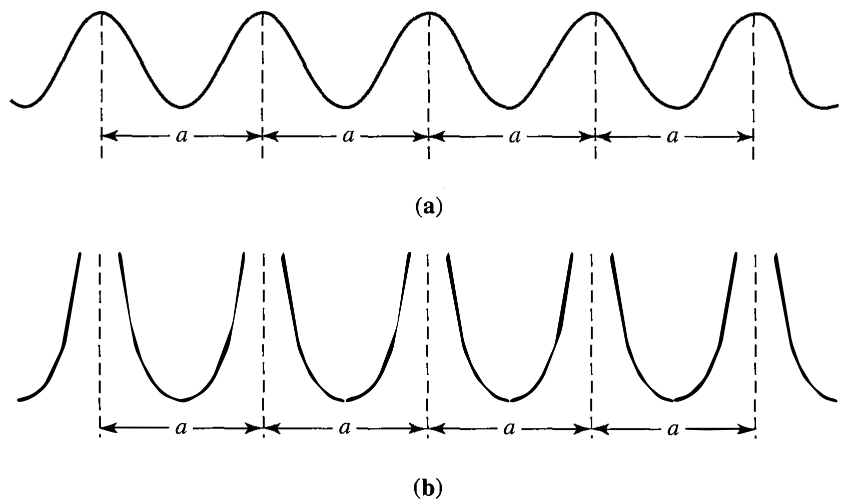
- Parity plays an important and fundamental role in the character of the states connected through an interaction.
- We can show that the parity-odd operator **r** connects only states of opposite parity. This has a very important consequence on radiative transitions between atomic states.

Lattice Translation as a Discrete Symmetry

- Consider a periodic potential in one dimension, where:

$$V(x \pm a) = V(x)$$

- A realistic example is the motion of an electron in a chain of regularly spaced positive ions.



(a) Periodic potential in one dimension with periodicity a. (b) The periodic potential when the barrier height between two adjacent lattice sites becomes infinite.

Lattice Translation as a Discrete Symmetry

- If the translation is represented by an operator $\tau(a)$, then we have:

$$\boldsymbol{\tau}^{+}\left(a\right)V(x)\boldsymbol{\tau}\left(a\right)=V(x\pm a)=V(x)$$

- Because the kinetic-energy part of the Hamiltonian is invariant under the translation with any displacement

$$\boldsymbol{\tau}^{+}\left(a\right)H\boldsymbol{\tau}\left(a\right)=H$$

- Since $\tau(a)$ is unitary we have

$$\left[H,\boldsymbol{\tau}\left(a\right)\right]=0$$

Lattice Translation as a Discrete Symmetry

- The previous relation shows that the Hamiltonian and the translation operator may have common eigenstates.
- We may show that in the case of infinite potential barriers these eigenstates are given from:

$$\left|\theta\right\rangle \equiv \sum_{n=-\infty}^{\infty} e^{in\theta}\left|n\right\rangle, \qquad -\pi \le \theta \le \pi$$

Lattice Translation as a Discrete Symmetry

- In the case of not-infinite barrier again we may consider the eigenstates:

$$|\theta\rangle \equiv \sum_{n=-\infty}^{\infty} e^{in\theta}|n\rangle, \qquad -\pi \le \theta \le \pi$$

- But now we need an assumption about states of different sites:

$$\langle n'|H|n\rangle \neq 0 \quad \text{only if } n' = n \quad \text{or} \quad n' = n+1$$

- This, in the solid-state physics, is the assumption known as **the tight-binding approximation**.

Lattice Translation as a Discrete Symmetry

- In this case the states $|\theta\rangle$ are Hamiltonian eigenstates with eigenvalues given by:

$$E_n = \left(E_0 - 2\Delta\cos\theta\right), \quad \text{with} \quad \Delta = -\left\langle n \pm 1 \middle| H \middle| n \right\rangle$$

- This, in the solid-state physics, is the assumption known as **the tight-binding approximation**.

Lattice Translation as a Discrete Symmetry

- It can be shown that for the wavefunction of $|\theta\rangle$, given as $\langle x|\theta\rangle$ we have:

$$\langle x|\theta\rangle = e^{ikx}u_k(x), \quad \theta = ka$$

- This the famous **Bloch Theorem** in solid state physics. Which states: *The eigenstates of a periodic potential can be always written as a product of an exponential function with a function which gas the periodicity of the potential.*

Lattice Translation as a Discrete Symmetry

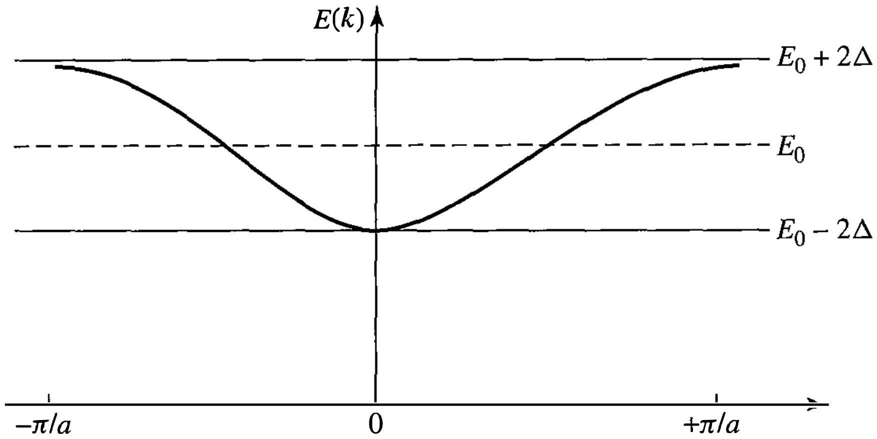
- These eigenstates look similar to the plane wave eigenfunctions $\psi_k(x) = Ae^{ikx}$ but with an amplitude having the periodicity of the potential.
- The most fascinating property is that there are no terms proportional to $\propto e^{-ikx}$. This means there is no possibility for the particle to be reflected in the opposite direction! The particle moves inside the potential with constant "momentum". The presence of the potential imposes just a spatial periodic modulation of the of the wave amplitude.

Lattice Translation as a Discrete Symmetry

- The only thing that changes is the dispersion relation from $E(k) = \hbar^2 k^2 / 2M$ of a free particle to

$$E(k) = E_0 - 2A\cos(ka)$$

for the particle in the periodic potential.



Dispersion curve for $E(k)$ versus k in the Brillouin zone $|k| \leq \pi/a$.

Lattice Translation as a Discrete Symmetry

- What is the physical meaning of θ? With the way it is defined the quantity k can considered as the momentum of the particle inside the periodic potential.
- This is not rigorously correct. Only the plane waves have a sharp momentum. The quantity k is not extended in the region $-\infty < k < \infty$ but only in the region $-\pi / a \leq k \leq +\pi / a$, the so called Brillouin zone.

Lattice Translation as a Discrete Symmetry

- In other words the motion of the particle “feels” no resistance at all! An external field can accelerate the particle up to a momentum at the limits of the relevant zone where reflections occur and the start the so called **Bloch oscillations.**
- For small momenta the particles move freely in the potential. The mean free path and the conductivity are infinite!
- Only deviations from the perfect periodicity (like impurities and defects) can delay the motion. This is what happens in a real conductor.