Advanced Quantum Physics
Week 2

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Fall 2019

# Symmetries in quantum mechanics

Identifying the symmetries of a system can be a very powerful tool to get insights into its physical properties. There are two kinds of symmetry groups: discrete symmetry groups (e.g. the benzene molecule is invariant under the discrete $C_6$ rotation group) and continuous symmetry groups, called *Lie groups* (e.g. the continuous rotations of a central potential problem). Emmy Noether has demonstrated that to every continuous symmetry there is an associated conserved physical quantity. For example, the conservation of energy is a consequence of time-translational invariance. Similarly, the conservation of momentum and angular momentum are consequences of translational and rotational invariance. In the following, we will see how Noether's theorem appears in quantum mechanics and how it can be used to help us solve the Schrödinger equation.

## Evolution operator

Let us start with the Schrödinger equation

$$i\hbar\frac{d}{dt}|\Psi(t)\rangle = \hat{\mathcal{H}}(t)|\Psi(t)\rangle$$

Because this is a first order differential equation in time, the state at a time $t$ is uniquely determined from the state at an earlier time $t_0$. This can be expressed by an operator acting on the state at time $t_0$

$$|\Psi(t)\rangle = \hat{U}(t,t_0)|\Psi(t_0)\rangle,$$

where $\hat{U}(t,t_0)$ is the *evolution operator* from time $t_0$ to time $t$. This operator has the following properties

- Clearly $\hat{U}(t,t) = \mathbb{1}$

- It is the solution of this equation
$$i\hbar\frac{\partial}{\partial t}\hat{U}(t,t_0) = \hat{\mathcal{H}}(t)\hat{U}(t,t_0),$$
with the initial condition $\hat{U}(t_0,t_0) = \mathbb{1}$.
- It is unitary, $\hat{U}(t,t')\hat{U}^\dagger(t,t') = \hat{U}^\dagger(t,t')\hat{U}(t,t') = \mathbb{1}$. Indeed,
$$\frac{\partial}{\partial t}\Big(\hat{U}^\dagger(t,t')\hat{U}(t,t')\Big) = \frac{i}{\hbar}\hat{U}^\dagger(t,t')\hat{\mathcal{H}}(t)\hat{U}(t,t') + \frac{-i}{\hbar}\hat{U}^\dagger(t,t')\hat{\mathcal{H}}(t)\hat{U}(t,t') = 0.$$
Given that $\hat{U}(t',t')\hat{U}(t',t') = \mathbb{1}$, we have that $\hat{U}^\dagger(t,t')\hat{U}(t,t') = \mathbb{1}$ for all times $t$. The same argument shows that $\hat{U}(t,t')\hat{U}^\dagger(t,t') = \mathbb{1}$.
- Composition: $\hat{U}(t_2,t_0) = \hat{U}(t_2,t_1)\hat{U}(t_1,t_0)$. Therefore $\hat{U}(t_0,t_1) = \hat{U}(t_1,t_0)^{-1}$.

If the Hamiltonian is time independent, as for an isolated system, then the evolution equation for $\hat{U}$ can be solved easily
$$\hat{U}(t,t_0) = \exp\Big(-i\frac{\hat{\mathcal{H}}}{\hbar}(t-t_0)\Big)$$
This result can also be obtained by remembering the time evolution of stationary states $|n\rangle$ of $\hat{\mathcal{H}}$
$$|\Psi(t)\rangle = \sum_n c_n(t_0)\exp\left(-i\frac{E_n}{\hbar}(t-t_0)\right)|n\rangle$$
where
$$c_n(t_0) = \langle n|\Psi(t_0)\rangle$$
Putting this back in the equation above
$$\begin{aligned}
|\Psi(t)\rangle &= \sum_n \langle n|\Psi(t_0)\rangle \exp\left(-i\frac{E_n}{\hbar}(t-t_0)\right)|n\rangle \\
&= \sum_n \left(\exp\left(-i\frac{E_n}{\hbar}(t-t_0)\right)|n\rangle\langle n|\right)|\Psi(t_0)\rangle \\
&= \sum_n \left(\exp\left(-i\frac{\hat{\mathcal{H}}}{\hbar}(t-t_0)\right)|n\rangle\langle n|\right)|\Psi(t_0)\rangle \\
&= \left(\exp\left(-i\frac{\hat{\mathcal{H}}}{\hbar}(t-t_0)\right)\sum_n |n\rangle\langle n|\right)|\Psi(t_0)\rangle \\
&= \exp\left(-i\frac{\hat{\mathcal{H}}}{\hbar}(t-t_0)\right)|\Psi(t_0)\rangle \\
&= \hat{U}(t,t_0)|\Psi(t_0)\rangle
\end{aligned}$$
We recognize that the expression for $\hat{U}(t,t_0)$ is the same as we have obtained above.

Note that in this case the time evolution operator clearly commutes with the Hamiltonian, $[\hat{\mathcal{H}},\hat{U}] = 0$ and the energy is conserved (we have proven that earlier). Phrased differently, we can say that because there is time translational symmetry, the time translation operator $\hat{U}$ commutes with the Hamiltonian and that this leads to the conservation of energy.

## Symmetry operators commute with the Hamiltonian

Let us suppose that the Hamiltonian of the system we consider is invariant under some symmetry operation $R$. There is an associated operator $\hat{\mathcal{R}}$ that is acting on kets

$$|\Psi'\rangle = \hat{\mathcal{R}}|\Psi\rangle,$$

where $|\Psi'\rangle$ is the image of $|\Psi\rangle$ under the action of the symmetry operator, e.g. a translation, a rotation, etc. The symmetry operator does not change the norm of the ket, it is unitary $\hat{\mathcal{R}}^\dagger\hat{\mathcal{R}} = \hat{\mathcal{R}}\hat{\mathcal{R}}^\dagger = \mathbb{1}$.

Let us emphasize that the state $|\Psi\rangle$ need not be symmetric, only the Hamiltonian. For example, the Hamiltonian may have time-translational symmetry (i.e. be time independent) but this does not imply that the state of the system $|\Psi(t)\rangle$ is time independent.

Rather, we expect that having a symmetry leads to the following property: If we start from a given state $|\Psi(t=0)\rangle$ at time $t=0$, the two situations below will lead to the same final state $|\Psi(t)\rangle$

- Start from $|\Psi(t=0)\rangle$. Act on it with the symmetry operator $\hat{\mathcal{R}}$ and then let it evolve until time $t$. This is described by

$$|\Psi(t)\rangle = \hat{U}(t,t_0)\hat{\mathcal{R}}|\Psi(t=0)\rangle$$

- Start from $|\Psi(t=0)\rangle$. Let it evolve until time $t$. Then act on it with the symmetry operator $\hat{\mathcal{R}}$. This is described by

$$|\Psi(t)\rangle = \hat{\mathcal{R}}\hat{U}(t,t_0)|\Psi(t=0)\rangle$$

Because the Hamiltonian is invariant under $R$, the evolution will be the same whether the initial state has been acted on by $\hat{\mathcal{R}}$ or not. We therefore have

$$[\hat{U}(t,t_0),\hat{\mathcal{R}}] = 0$$

Let us expand $\hat{U}$

$$\hat{U}(t+\Delta t,t) = \hat{U}(t,t) + \Delta t\frac{d\hat{U}}{dt} = \mathbb{1} + \Delta t\big(-\frac{i}{\hbar}\big)\hat{\mathcal{H}}\hat{U}(t,t) = \mathbb{1} + \Delta t\big(-\frac{i}{\hbar}\big)\hat{\mathcal{H}}$$

It is therefore clear that if $\hat{U}(t',t)$ and $\hat{\mathcal{R}}$ commute for all $t,t'$, then also the Hamiltonian commutes with $\hat{\mathcal{R}}$

$$[\hat{\mathcal{H}},\hat{\mathcal{R}}] = 0.$$

This is an important result. It shows that the operators associated to a symmetry of the system commute with the Hamiltonian. This has two immediate consequences

- The average value $\langle\Psi(t)|\hat{\mathcal{R}}|\Psi(t)\rangle$ is constant in time. This comes directly from the Ehrenfest theorem. Alternatively one can see that

$$\begin{aligned}\langle\Psi(t)|\hat{\mathcal{R}}|\Psi(t)\rangle &= \langle\Psi(t_0)|\hat{U}^\dagger(t,t_0)\hat{\mathcal{R}}\hat{U}(t,t_0)|\Psi(t_0)\rangle \\ &= \langle\Psi(t_0)|\hat{U}^\dagger(t,t_0)\hat{U}(t,t_0)\hat{\mathcal{R}}|\Psi(t_0)\rangle = \langle\Psi(t_0)|\hat{\mathcal{R}}|\Psi(t_0)\rangle\end{aligned}$$

- There is a basis where both the Hamiltonian $\hat{\mathcal{H}}$ and $\hat{\mathcal{R}}$ are diagonal.

This is close to Noether's theorem but one has to keep in mind that $\hat{\mathcal{R}}$ is not an observable. It is unitary, but not Hermitian in general. There is therefore one more step to take.

## Noether's theorem

The results above are general for any kind of symmetry. Let us now focus on continuous symmetries (mathematically described by Lie groups). These symmetries can be parametrized by a continuous parameter $a$ and we can write the action of the symmetry operator as $\hat{\mathcal{R}}_a$. Let us then consider the action of an infinitesimal step of the symmetry operator

$$\hat{\mathcal{R}}_{\delta a} = \mathbb{1} - \frac{i}{\hbar}\hat{G}\delta a$$

The adjoint operator satisfies

$$\hat{\mathcal{R}}^{\dagger}_{\delta a} = \mathbb{1} + \frac{i}{\hbar}\hat{G}^{\dagger}\delta a$$

In these equation, the operator $\hat{G}$ is called the infinitesimal generator of the symmetry. It is obtained from a derivative with respect to $a$ of the symmetry operator

$$\hat{G} = \frac{\hbar}{i}\frac{\partial \hat{\mathcal{R}}_a}{\partial a}(a = 0)$$

From the expressions above, it immediately follows that because $\hat{\mathcal{R}}_a$ is unitary, the operator $\hat{G}$ is Hermitian $\hat{G} = \hat{G}^{\dagger}$. It also commutes with the Hamiltonian

$$[\hat{G}, \hat{\mathcal{H}}] = 0$$

Given that $\hat{G}$ is Hermitian it is associated to a physical quantity that is conserved. This is the expression of Noether's theorem in the context of quantum mechanics: the infinitesimal generators of a symmetry group are constants of motion. We will see below that for example the momentum operator is the infinitesimal generator of translations and that momentum is conserved in translationally-invariant systems.

## A simple example: the parity

Let us consider a system that is invariant under a parity operation $x \to -x$. There are many examples: symmetric potential wells, the harmonic oscillator, the benzene molecule. The corresponding operator acts on kets as follows

$$\left(\hat{\Pi}\Psi\right)(x) = \Psi(-x)$$

The operator has the following properties

- Hermitian: $\hat{\Pi}^{\dagger} = \hat{\Pi}$
- Unitary: $\hat{\Pi}^{\dagger}\hat{\Pi} = \hat{\Pi}\hat{\Pi}^{\dagger} = \mathbb{1}$
- Involution: $\hat{\Pi}^2 = \mathbb{1}$

As we have seen above, if the system has inversion symmetry then

$$[\hat{\Pi}, \hat{\mathcal{H}}] = 0$$

and there is a basis that diagonalizes both operators. Because $\hat{\Pi}$ is an involution, its two possible eigenvalues are $\pm 1$. The eigenstates can therefore be classified between those that are symmetric under inversion and those that are antisymmetric

$$\begin{aligned} \hat{\Pi}|\Psi_S\rangle &= +|\Psi_S\rangle \qquad \text{symmetric} \\ \hat{\Pi}|\Psi_A\rangle &= -|\Psi_A\rangle \qquad \text{antisymmetric} \end{aligned}$$

One can remember some one-dimensional systems that had inversion symmetry, such as the harmonic oscillator, and see that indeed the eigenstates are either symmetric or antisymmetric.

## Continuous translations

Let us now consider a system that has a continuous translation symmetry. It is described by an operator $\hat{T}_a$

$$\begin{aligned}\big(\hat{T}_a\Psi\big)(x) &= \Psi(x-a)\\ \langle x|\hat{T}_a|\Psi\rangle &= \langle x-a|\Psi\rangle,\end{aligned}$$

which also means, quite naturally, that $\hat{T}_a|x_0\rangle = |x_0+a\rangle$. The translation operator is unitary $\hat{T}_a^\dagger\hat{T}_a = \hat{T}_a\hat{T}_a^\dagger = \mathbb{1}$. This property ensures that it can be diagonalized. Note however that $\hat{T}_a$ is not Hermitian and therefore does not need to have real eigenvalues.

Let us investigate the effect of an infinitesimal translation on a state $|\Psi\rangle$

$$\begin{aligned}\big(\hat{T}_{\delta a}\Psi\big)(x) &= \Psi(x-\delta a) = \Psi(x) - \delta a\frac{\partial\Psi}{\partial x}\\ &= \Big(\mathbb{1} - \frac{i}{\hbar}\delta a\frac{\hbar}{i}\frac{\partial}{\partial x}\Big)\Psi(x)\end{aligned}$$

This allows to make the connection with the momentum operator $\hat{p}$

$$\begin{aligned}\hat{T}_{\delta a}|\Psi\rangle &= \Big(\mathbb{1} - \frac{i}{\hbar}\delta a\hat{p}\Big)|\Psi\rangle\\ \hat{T}_{\delta a} &= \mathbb{1} - \frac{i}{\hbar}\hat{p}\delta a\end{aligned}$$

We see that $\hat{p}$ can be seen as an infinitesimal generator of translations. Also note how this is reminiscent of the expression for an infinitesimal time evolution obtained above.

The translation operator obeys the natural composition rule

$$\hat{T}_{a+\delta a} = \hat{T}_{\delta a}\hat{T}_a$$

Using a Taylor expansion on the left and the result for an infinitesimal translation on the right, we obtain

$$\begin{aligned}\hat{T}_a + \delta a\frac{\partial\hat{T}_a}{\partial x} &= \Big(\mathbb{1} - \frac{i}{\hbar}\hat{p}\delta a\Big)\hat{T}_a\\ \frac{\partial\hat{T}_a}{\partial x} &= -\frac{i}{\hbar}\hat{p}\hat{T}_a\end{aligned}$$

Solving this equation yields the following important result

$$\hat{T}_a = \exp\Big(-\frac{i}{\hbar}\hat{p}a\Big)$$

Note again the similarity with the expression for the time evolution operator in the case when the Hamiltonian was time independent.

## A new definition of the momentum

The results above allow to give a new definition of the momentum operator: *The momentum operator is the infinitesimal generator of the translation group.* Generalized to three dimensions this reads

$$\hat{T}_{\delta\vec{a}} = \mathbb{1} - \frac{i}{\hbar}\hat{\vec{p}} \cdot \delta\vec{a}$$

## Translationally invariant systems

If a system is described by a translationally invariant Hamiltonian, we have

$$[\hat{T}_a, \hat{\mathcal{H}}] = 0 \rightarrow [\hat{T}_{\delta a}, \hat{\mathcal{H}}] = 0 \rightarrow [\mathbb{1} - \frac{i}{\hbar}\hat{p}\delta a, \hat{\mathcal{H}}] = 0$$

Therefore the Hamiltonian commutes with the momentum operator

$$[\hat{p}, \hat{\mathcal{H}}] = 0$$

This has the important consequences that

- <u>Momentum is conserved</u> (Ehrenfest theorem)
- $\hat{p}$ and $\hat{\mathcal{H}}$ can be diagonalized together

The eigenstates of $\hat{p}$ are plane waves

$$\langle x|p\rangle = \frac{e^{ipx/\hbar}}{2\pi\hbar}$$
$$\hat{p}|p\rangle = p|p\rangle$$

If the Hamiltonian has translational symmetry, then the potential $V(x) = \text{const}$ must be uniform

$$\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m}$$

It is clear that $|p\rangle$ is indeed an eigenstate of the Hamiltonian

$$\hat{\mathcal{H}}|p\rangle = \frac{p^2}{2m}|p\rangle$$

Finally, let us verify that the action of $\hat{T}_a$ is indeed the one we expect from

$$\hat{T}_a = \exp\left(-\frac{i}{\hbar}\hat{p}a\right)$$

We have that

$$\hat{T}_a e^{ipx/\hbar} = e^{ip(x-a)/\hbar} = e^{-ipa/\hbar}e^{ipx/\hbar}$$
$$\hat{T}_a|p\rangle = e^{-ipa/\hbar}|p\rangle$$

which is indeed compatible with the expression above.

# Discrete translations

Here we will focus on the group of discrete translations. This group is relevant to describe systems such as crystals that are invariant under the action of translations that link two equivalent atoms. We will show that in that case, the wave functions do not need to be plane waves as in the case of continuous translations, but nevertheless have a structure which is very reminiscent of plane waves. This is expressed by a theorem due to Felix Bloch.

## Bloch theorem

We consider a particle in a one-dimensional periodic potential $V(x)$. The periodicity of the potential is $a$ such that $V(x+a) = V(x)$. It is described by the Hamiltonian

$$\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + V(\hat{x})$$

The system is invariant under a translation $a$ described by the operator $\hat{T}_a$. As discussed above, this has the consequence

$$[\hat{\mathcal{H}}, \hat{T}_a] = 0$$

Because $\hat{\mathcal{H}}$ and $\hat{T}_a$ commute, they have a common set of eigenvectors. The translation operator $\hat{T}_a$ is unitary $\hat{T}_a\hat{T}_a^\dagger = \hat{T}_a^\dagger\hat{T} = \mathbb{1}$ and is therefore diagonalizable

$$\hat{T}_a|\Psi_k\rangle = \lambda_k|\Psi_k\rangle$$

Because $\hat{T}_a$ is unitary, the eigenvalues $\lambda_k$ must satisfy $|\lambda_k| = 1$ and they can be written as $\lambda_k = \exp(-ika)$ with $k \in [-\pi/a, \pi/a[$. Indeed any value of $k$ outside this interval is redundant with one of the values in the interval.

### Bloch theorem - version 1

The result above allows to formulate a first version of Bloch's theorem: If a system is described by a periodic potential of period $a$, its eigenvectors $|\Psi_k\rangle$ can be chosen such that

$$\hat{T}_a|\Psi_k\rangle = e^{-ika}|\Psi_k\rangle,$$

with $k \in [-\pi/a, \pi/a[$.

### Bloch theorem - version 2

Let us introduce the function $u_k(x)$ such that

$$\Psi_k(x) = e^{ikx}u_k(x)$$

By acting with the translation operator on both sides we obtain

$$\hat{T}_a\Psi_k(x) = e^{-ika}\Psi_k(x) = e^{-ika}e^{ikx}u_k(x)$$
$$\hat{T}_a e^{ikx}u_k(x) = e^{ik(x-a)}u_k(x-a) = e^{-ika}e^{ikx}u_k(x-a)$$

We conclude that $u_k(x)$ has to be a periodic function $u_k(x) = u_k(x - a)$. This allows to state the second version of Bloch's theorem: The eigenstates of a system described by a periodic potential of period $a$ can always be written as

$$\Psi_k(x) = e^{ikx} u_k(x),$$

where $u_k(x)$ is a periodic function of period $a$. One can see from this expression that the eigenstates take the form of a plane wave multiplied by a periodic function. Because these are not exactly plane waves, $k$ is not exactly the momentum of the particle. But one can show that it has nevertheless many similarities with the momentum operator.

## Noether's theorem for discrete symmetries?

So what happens to Noether's theorem in cases when the symmetry of the system is discrete? It turns out that there is still some kind of conservation law for discrete symmetries. When the symmetry group is infinite, such as the translations of the crystal, there is a conserved quantity but it is periodic. For example, in a crystal momentum is conserved modulo vectors in the reciprocal lattice. If the group is finite the conserved quantities are discrete and in general lead to selection rules which tell what processes are allowed.