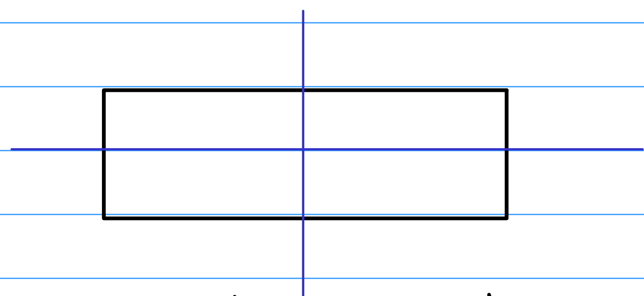
Symmetries in QM

Let us start with spatial symmetries, which are intuitive.

To decide whether a given object has a symmetry we must (i) Define a transformation that can act on any object (ii) Let it act on the object of interest (iii) If the transformed object is the same as the original, the object is symmetric under the given transformation.

Take the example of a rectangle with unequal sides.



Consider the transformation which corresponds to reflecting around the vertical blue line. The rectangle is symmetric under this transformation

Another transformation is rotation by $\pi/2$ counterclockwise. The rectangle is not symmetric under this transformation.

In QM symmetry transformations act on states in the Hilbert space. One should think of any such transformation as the generalization of rotations which leave inner products unchanged.

So Symmetry transformations correspond to Unitary operators on the states.

Symmetries typically form a mathematical structure called a Group, which embodies the abstract idea of multiplication and division without talking about addition and subtraction.

A group G has elements $g \in G$ which satisfy

(i) There is a group multiplication

$$\boxed{\text{If } \quad g_1, g_2 \in G \quad \text{then} \quad g_1 \cdot g_2 \in G} \quad (1)$$

Closed under multiplication

Note that multiplication need not be commutative but must be associative

$$\boxed{g_1 \cdot (g_2 \cdot g_3) = (g_1 \cdot g_2) \cdot g_3} \quad (2)$$

(ii) There is a unique identity element $e \in G$ such that

$$\boxed{e \cdot g = g \cdot e = g \quad \forall\, g \in G} \quad (3)$$

(iii) Every element has a unique inverse

$$\boxed{\begin{array}{l} \text{If } \quad g \in G \quad \exists \; g^{-1} \in G \quad \text{such that} \\ \qquad g \cdot g^{-1} = g^{-1} \cdot g = e \end{array}} \quad (4)$$

Groups in which all elements commute are called Abelian while the rest are called non-Abelian.

For the rectangle we considered the symmetry operations are

e = leave the object alone (identity transformation)

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R_x = reflection $x \to -x$ around the vertical blue line

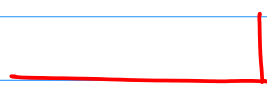
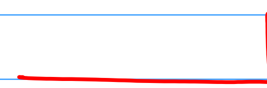
R_y = reflection $y \to -y$ around the horizontal blue line

C_2 = rotation around the center by $\pm\pi$

To see the complete group this corresponds to one must act on a non-symmetric object.

For example

C_2  = 

$R_x C_2$  = $= C_2 R_x$ 

So R_x and C_2 commute but $R_x C_2$ is another element of the group. Similarly

$R_y C_2 = C_2 R_y$ is yet another element.

However $R_x R_y = R_y R_x$ is not a new element but is simply C_2. Also

$$C_2^2 = C_2 \cdot C_2 = e = R_x^2 = R_y^2$$

An important role of symmetry in QM has been to classify eigenstates of Hamiltonians.

Suppose one has a group of transformations G that act on a physical system. They are said to be represented in the Hilbert space $\mathcal{V}$ by a group of Unitary operators (matrices) where group multiplication maps to matrix multiplication

$$\boxed{g \in G \to \mathbb{U}(g) = \text{Unitary operators acting on } \mathcal{V}} \quad (6)$$

$$\boxed{g_1 \circ g_2 = g_3 \Rightarrow \quad \mathbb{U}(g_1)\,\mathbb{U}(g_2) = \mathbb{U}(g_3)} \quad (7)$$

$$\boxed{\mathbb{U}(e) = \mathbb{1} \quad \text{and} \quad \mathbb{U}(g^{-1}) = (\mathbb{U}(g))^{-1} = (\mathbb{U}(g))^{\dagger}} \quad (8)$$

If the Hamiltonian $\mathcal{H}$ is symmetric under the transformations then

$$\boxed{[\mathcal{H}, \mathbb{U}(g)] = 0 \qquad \forall g \in G} \quad (9)$$

This has been pretty abstract so far. Let's consider specific examples

Example 1: Translation invariance. Consider N interacting particles subject to the Hamiltonian

$$\boxed{\mathcal{H} = \sum_{a=1}^{N} \frac{\vec{\mathbb{P}}_a^{\,2}}{2M_a} + \sum_{a<b} V_{ab}(\vec{\mathbb{X}}_a - \vec{\mathbb{X}}_b)} \quad (10)$$

The transformation $\boxed{\vec{x}_a \to \vec{x}_a + \bar{R} \quad \forall a}$ (11) is a symmetry because it does not change $\vec{x}_a - \vec{x}_b$.

What is the unitary operator that implements this symmetry on states? It is simply

$$\boxed{\mathbb{U}(\bar{R}) = \exp\left\{ \frac{i}{\hbar} \bar{R} \cdot \sum_{a=1}^{N} \vec{\mathbb{P}}_a \right\}} \quad (12)$$

Consider first its action on a wavefunction

$$\vec{\mathbb{P}}_a \to -i\hbar \vec{\nabla}_a$$

$$\boxed{\mathbb{U}(\bar{R}) \Psi(\{\vec{x}_a\}) = e^{\bar{R} \cdot \sum \vec{\nabla}_a} \Psi(\{\vec{x}_a\}) = \Psi(\{\vec{x}_a + \bar{R}\})} \quad (13)$$

To see that $\mathbb{U}(\bar{R})$ commutes with $\mathcal{H}$ all we need do is consider its action on $\vec{x}_b$

$$\boxed{\mathbb{U}(\bar{R})\, f(\vec{x}_b)\, |\Psi\rangle = \mathbb{U}(\bar{R}) f(\vec{x}_b) \mathbb{U}^\dagger(\bar{R})\ \mathbb{U}(\bar{R}) |\Psi\rangle} \quad (14)$$

So, when acting on the symmetry-transformed states

$$\boxed{\begin{aligned} f(\vec{x}_b) &\to \mathbb{U}(\bar{R}) f(\vec{x}_b) \mathbb{U}^\dagger(\bar{R}) \\ &= f\left(\mathbb{U}(\bar{R})\, \vec{x}_b\, \mathbb{U}^\dagger(\bar{R})\right) \end{aligned}} \quad (15)$$

Now consider

$$\boxed{\vec{\mathbb{F}}_b(\bar{R}) = \mathbb{U}(\bar{R})\, \vec{x}_b\, \mathbb{U}^\dagger(\bar{R})} \quad (16)$$

$$\mathbb{F}_{bi}(\bar{R}) = e^{\frac{i}{\hbar}\bar{R}\cdot\bar{\mathbb{P}}_b} \mathbb{X}_{bi}\, e^{-\frac{i}{\hbar}\bar{R}\cdot\bar{\mathbb{P}}_b}$$

$$\frac{\partial \mathbb{F}_{bi}}{\partial R_j} = \frac{i}{\hbar}\, e^{\frac{i}{\hbar}\bar{R}\cdot\bar{\mathbb{P}}_b} \underbrace{[\mathbb{P}_{bj}, \mathbb{X}_{bi}]}_{-i\hbar\delta_{ij}} e^{-\frac{i}{\hbar}\bar{R}\cdot\bar{\mathbb{P}}_b}$$

$$\frac{\partial \mathbb{F}_{bi}}{\partial R_j} = \delta_{ij} \Rightarrow \quad \mathbb{F}_{bi}(\bar{R}) = \mathbb{F}_{bi}(0) + R_i$$
$$= \mathbb{X}_{bi} + R_i$$

In short

$$\boxed{\mathbb{U}(\bar{R})\bar{\mathbb{X}}_b\mathbb{U}^\dagger(\bar{R}) = \bar{\mathbb{X}}_b + \bar{R}} \quad (17)$$

So
$$\boxed{\mathbb{U}(\bar{R})\, V_{ab}(\bar{\mathbb{X}}_a - \bar{\mathbb{X}}_b)\, \mathbb{U}^\dagger(\bar{R}) = V_{ab}(\bar{\mathbb{X}}_a + \bar{R} - \bar{\mathbb{X}}_b - \bar{R}) = V_{ab}(\bar{\mathbb{X}}_a - \bar{\mathbb{X}}_b)} \quad (18)$$

$$\Rightarrow \boxed{\mathbb{U}(\bar{R})\,\mathbb{H}\,\mathbb{U}^\dagger(\bar{R}) = \mathbb{H}} \quad (19)$$

Multiply from the right by $\mathbb{U}(\bar{R})$

$$\Rightarrow \boxed{\mathbb{U}(\bar{R})\mathbb{H} = \mathbb{H}\,\mathbb{U}(\bar{R}) \Rightarrow \quad [\mathbb{H}, \mathbb{U}(\bar{R})] = 0} \quad (20)$$

Note that $\bar{R}$ can be any vector. The full group is labelled by $\bar{R}$, so it has an uncountably infinite number of elements.

$\boxed{\bar{R} = 0 \text{ corresponds to the identity}}$ (21)

$\boxed{\text{For } g = \bar{R} \quad g^{-1} = -\bar{R}}$ (22)

The group is abelian

$$\boxed{\mathbb{U}(\bar{R}_1)\,\mathbb{U}(\bar{R}_2) = \mathbb{U}(\bar{R}_1+\bar{R}_2)} \quad (23)$$

Since $[\mathbb{U}(\bar{R}), \mathcal{H}] = 0 = [\mathbb{U}(\bar{R}_1), \mathbb{U}(\bar{R}_2)]$ we can simultaneously diagonalize $\mathbb{U}(\bar{R})$ and $\mathcal{H}$.

Consider eigenstates of a unitary operator $\mathbb{U}$

$$\boxed{\begin{aligned} \mathbb{U}\,|\alpha\rangle &= u_\alpha|\alpha\rangle \\ \langle\alpha|\,\mathbb{U}^\dagger &= u_\alpha^*\langle\alpha| \end{aligned}} \quad (24)$$

$$\Rightarrow \quad \langle\alpha|\,\mathbb{U}^\dagger\,\mathbb{U}\,|\alpha\rangle = |u_\alpha|^2$$

But $\mathbb{U}^\dagger\mathbb{U} = \mathbb{1}$ so $\boxed{|u_\alpha|^2 = 1.}$ (25)

The eigenvalues of a unitary matrix are of the form

$$\boxed{u_\alpha = e^{i\theta_\alpha}} \quad (26) \qquad \text{unimodular.}$$

Back to our problem. Let us consider a simultaneous eigenstate of $\mathbb{U}(\bar{R}_1)$, $\mathbb{U}(\bar{R}_2)$

$$\boxed{\mathbb{U}(\bar{R}_1)\,|\alpha\rangle = e^{i\theta(\bar{R}_1)}|\alpha\rangle \qquad \mathbb{U}(\bar{R}_2)\,|\alpha\rangle = e^{i\theta(\bar{R}_2)}|\alpha\rangle} \quad (27)$$

$$\mathbb{U}(\bar{R}_1)\,\mathbb{U}(\bar{R}_2) = \mathbb{U}(\bar{R}_1+\bar{R}_2)$$

$$\Rightarrow \quad \boxed{\theta(\bar{R}_1+\bar{R}_2) = \theta(\bar{R}_1) + \theta(\bar{R}_2)} \quad (28)$$

so θ must be a linear function of $\bar{R}$. The most general linear function is

$$\boxed{\theta(\bar{R}) = \frac{1}{\hbar}\bar{P}\cdot\bar{R}} \quad (29)$$

$\bar{P}$ is a constant with units of momentum.

So the simultaneous eigenstates of $\mathbb{H}$ and $\mathbb{U}(\bar{R})$ can be labelled by a vector $\bar{P}$. Of course, there will be additional labels, which we call μ

$$\Rightarrow \quad \boxed{\mathbb{U}(\bar{R})\,|\bar{P},\mu\rangle = e^{\frac{i}{\hbar}\bar{P}\cdot\bar{R}}\,|\bar{P},\mu\rangle} \quad (30)$$

What is the physical meaning of $\bar{P}$? Recall the definition of $\mathbb{U}(\bar{R})$

$$\boxed{\mathbb{U}(\bar{R}) = \exp\left\{\frac{i}{\hbar}\bar{R}\cdot\sum_{a=1}^{N}\vec{\mathbb{P}}_a\right\}} \quad (12)$$

Now let us consider $\bar{R}$ to be infinitesimal.

$$\Rightarrow \quad \boxed{\mathbb{U}(\delta\bar{R}) \approx \left(1 + \frac{i}{\hbar}\delta\bar{R}\cdot\sum_{a=1}^{N}\vec{\mathbb{P}}_a + \cdots\right)} \quad (31)$$

(32)

Since $$\boxed{\mathbb{U}(\delta\bar{R})\,|\bar{P},\mu\rangle = e^{\frac{i\bar{P}\cdot\delta\bar{R}}{\hbar}}\,|\bar{P},\mu\rangle \approx \left(1 + \frac{i\,\delta\bar{R}\cdot\bar{P}}{\hbar} + \cdots\right)|\bar{P},\mu\rangle}$$

we conclude that

$$\boxed{\left(\sum_{a=1}^{N}\vec{\mathbb{P}}_a\right)|\bar{P},\mu\rangle = \bar{P}\,|\bar{P},\mu\rangle} \quad (33)$$

So $\bar{P}$ is simply the total momentum of all the particles, which is a conserved quantity.

Groups in which the group elements are labelled by continuous parameters such as $\bar{R}$ are called continuous groups or Lie groups.

In any Lie group one can make a lot of progress by taking transformations infinitesimally close to the identity. Suppose the group elements are labelled by "coordinates" $\lambda_1, \cdots \lambda_M$, then

$$\boxed{\mathbb{U}(g) = \mathbb{U}(\lambda_1, \cdots \lambda_M)} \quad (34)$$

is the unitary operator acting on the Hilbert space $\mathcal{V}$ representing g.

Choose the coordinates such that

$$\boxed{\lambda_1 = \lambda_2 \cdots = 0 \quad \text{corresponds to} \quad e} \quad (35)$$

$$\boxed{\mathbb{U}(e) = \mathbb{U}(\{\lambda_i = 0\}) = \mathbb{1}} \quad (36)$$

For small $\lambda_i = \delta\lambda_i$ (37)

$$\boxed{\mathbb{U}(\{\delta\lambda_i\}) = \mathbb{1} + i\,\delta\lambda_i\, \mathbb{A}_i + \cdots}$$

(implicit sum on i)

Can you see why $\mathbb{A}_i^\dagger = \mathbb{A}_i$?

The $\mathbb{A}_i$ are hermitian operators acting on $\mathcal{V}$ called the generators of the group of transformations

The reason they generate all transformations is that one can get to a transformation with finite $\{\lambda_i\}$ by applying the infinitesimal transformations many times.

In our example, the total momentum is the generator of translations.

Example 2: Discrete translation symmetry & Bloch's Theorem

Consider a particle moving in a periodic potential in, say, a perfect crystal.

$$\boxed{\mathcal{H} = \frac{\vec{\mathbb{P}}^2}{2M} + V(\vec{x})} \quad (38)$$

with $$\boxed{V(\vec{x}+\vec{a}_1) = V(\vec{x}+\vec{a}_2) = V(\vec{x}+\vec{a}_3) = V(\vec{x})} \quad (39)$$

here $\vec{a}_1, \vec{a}_2, \vec{a}_3$ are called the primitive lattice translation vectors. They are the smallest vectors by which you can translate the crystal and make it coincide with itself.

For a simple cubic lattice

$$\boxed{\vec{a}_1 = a\,\hat{e}_x \qquad \vec{a}_2 = a\,\hat{e}_y \qquad \vec{a}_3 = a\,\hat{e}_z} \quad (40)$$

Clearly, if $\boxed{\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3}$ (41) n_1, n_2, n_3 integer

then $$\boxed{V(\vec{x}+\vec{R}) = V(\vec{x})} \quad (42)$$

Now, this is similar to example 1, except for a crucial distinction. We no longer have a continuous group. Instead, we have a discrete group of translations.

$$\boxed{\mathbb{U}(\bar{R}) = e^{\frac{i}{\hbar}\bar{R}\cdot\bar{\mathbb{p}}}} \quad (43)$$

but now $\bar{R} = n_1\bar{a}_1 + n_2\bar{a}_2 + n_3\bar{a}_3$

n_i integer.

We cannot make $\bar{R}$ infinitesimal! Let us see how much progress we can make.

The group is still abelian

$$\boxed{\begin{gathered}[\mathbb{U}(\bar{R}), \mathbb{U}(\bar{R}')] = 0 \\ [\mathbb{U}(\bar{R}), \mathcal{H}] = 0\end{gathered}} \quad (44)$$

$\bar{R} = n_1\bar{a}_1 + n_2\bar{a}_2 + n_3\bar{a}_3$

Once again consider eigenstates of $\mathbb{U}(\bar{R})$. The eigenvalues must be unimodular

$$\boxed{\mathbb{U}(\bar{R})|\alpha\rangle = e^{i\theta_\alpha(\bar{R})}|\alpha\rangle} \quad (45)$$

$$\boxed{\mathbb{U}(\bar{R}_1)\,\mathbb{U}(\bar{R}_2) = \mathbb{U}(\bar{R}_1+\bar{R}_2) \Rightarrow \quad \theta_\alpha(\bar{R}_1) + \theta_\alpha(\bar{R}_2) = \theta_\alpha(\bar{R}_1+\bar{R}_2)} \quad (46)$$

θ_α is a linear function of $\bar{R}$

$$\Rightarrow \boxed{\theta_{\bar{k}}(\bar{R}) = \bar{k}\cdot\bar{R}} \quad (47)$$

$\bar{k}$ has units of wavevector

The eigenstates are labelled by $\bar{k}$ and some other index, say μ

$$\boxed{\begin{gathered}\mathbb{U}(\bar{R})|\bar{k},\mu\rangle = e^{i\bar{k}\cdot\bar{R}}|\bar{k},\mu\rangle \\ \mathcal{H}|\bar{k},\mu\rangle = \varepsilon_\mu(\bar{k})|\bar{k},\mu\rangle\end{gathered}} \quad (48)$$

This is Bloch's Theorem

Because $\bar{R} = n_1 \bar{a}_1 + n_2 \bar{a}_2 + n_3 \bar{a}_3$ there are some redundancies in $\bar{k}$. Let us specialize to the cubic lattice

$$\bar{a}_1 = a\hat{e}_x \qquad \bar{a}_2 = a\hat{e}_y \qquad \bar{a}_3 = a\hat{e}_z$$

$$\boxed{\text{If} \quad \bar{k}' = \bar{k} + \frac{2\pi}{a}\hat{e}_x \quad \text{then} \quad e^{i\bar{k}'\cdot\bar{R}} = e^{i\bar{k}\cdot\bar{R}}} \tag{49}$$

so $\bar{k}'$ corresponds to the same eigenvalue of $U(\bar{R})$ as $\bar{k}$.

$$\Rightarrow \boxed{\vec{k} \text{ is only defined mod } \frac{2\pi}{a}} \text{ in any direction} \tag{50}$$

One common choice is

$$\boxed{-\frac{\pi}{a} \leq k_x, k_y, k_z \leq \frac{\pi}{a}} \tag{51}$$

$\bar{k}$ is called the crystal momentum or pseudomomentum of the particle.

The quantum number μ is discrete and is called the band index. A single-particle state in a perfect crystal is specified by its crystal momentum and band index.

The next important spatial symmetry group is 3D rotations and we will spend quite a bit of time on them.