Chapter 5

Symmetries and Unitary Groups

In this chapter, we turn our attention to the realisation of *symmetries* in quantum theories/systems. Before developing a formal theory of quantum symmetry, we will look at a simple example that illustrates many features of the formalism and most of the key ideas.

5.1 An appetizer: spatial and time translations

Consider a particle moving freely (subject to no forces) on the real line (so, as in Chapter 1.3, the Hilbert space is identified as $\mathcal{H} \cong L^2(\mathbb{R})$, and additionally the Hamiltonian is just $H = P^2/2m$). There is an intuitive sense in which *linear translations* in space should be symmetries of the theory. How does this manifest in the quantum mechanical formalism?

For $a \in \mathbb{R}$, we can define an operator $T(a) : \mathcal{H} \to \mathcal{H}$ that corresponds to a translation of the entire system by a relative to a fixed reference frame. This will act on wavefunctions according to

$$(T(a)\psi)(x) = \psi(x-a) \ . \tag{5.1}$$

To understand why the minus sign, observe that the value of the transformed wavefunction at a will be the value of the original wave function at the origin. In terms of our generalised position eigenstates, we have[32]

$$T(a)\,|\xi\rangle = |\xi + a\rangle \ , \tag{5.2}$$

because a (generalised) eigenstate that was previously localised at $x = \xi$ should be localised at $x = \xi + a$ after translation. We see this is equivalent to (5.1) as follows,

$$\begin{aligned}
(T(a)\psi)(x) = \langle x|T(a)|\psi\rangle &= \int_{-\infty}^{\infty} \mathrm{d}\xi \ \langle x|T(a)|\xi\rangle \, \langle \xi|\psi\rangle \ , \\
&= \int_{-\infty}^{\infty} \mathrm{d}\xi \ \langle x|\xi + a\rangle \ \psi(\xi) \ , \\
&= \int_{-\infty}^{\infty} \mathrm{d}\xi \, \delta(x - \xi - a)\psi(\xi) \ , \\
&= \psi(x-a) \ .
\end{aligned} \tag{5.3}$$

We make some immediate observations regarding the structural properties of these translation operators:

(1) $T(a)T(b) = T(a+b) \quad \forall\, a, b \in \mathbb{R}$,

(2) $T(a)^{-1} = T(-a) \qquad \forall\, a \in \mathbb{R}$,

(3) $T(0) = 1$.

We can also determine the adjoint of this translation operator by a change of variables in the integral expression for the inner product,

$$\langle \chi|T(a)\psi\rangle = \int_{-\infty}^{\infty} \mathrm{d}x\, \chi(x)\psi(x-a) = \int_{-\infty}^{\infty} \mathrm{d}x\, \chi(x+a)\psi(x) = \langle T(-a)\chi|\psi\rangle \ . \tag{5.4}$$

[32] Keeping track of the signs here is a good exercise in disambiguating generalised position eigenstates from their wavefunctions

so we have

(4) $T(a)^* = T(-a) = T(a)^{-1}$

As in our discussion of time translation, this last condition identifies the operators $T(a)$ as unitary operators. The four properties that we have listed then precisely identify this structure as a *unitary representation of the additive group* $(\mathbb{R},+)$ *on the Hilbert space* $\mathcal{H}$.

Definition 5.1.1. The *unitary group* $\mathsf{U}(\mathcal{H})$ is the group of unitary operators on the Hilbert space $\mathcal{H}$. For the case of when $\mathcal{H}$ is finite-dimensional (say $\dim(\mathcal{H}) = n$), this can be identified with the usual matrix group $U(n)$.

Definition 5.1.2. A *unitary representation* of a group $\mathcal{G}$ on a Hilbert space $\mathcal{H}$ is a group homomorphism from $\mathcal{G}$ to $\mathsf{U}(\mathcal{H})$.

In the case of infinite-dimensional $\mathcal{H}$, such a group homomomorphism is required to be what is called *strongly continuous*. We will not need to pay attention to that restriction in this course and so will not define it carefully—what it means is that for any $\psi \in \mathcal{H}$, the induced map from $\mathcal{G}$ to $\mathcal{H}$ is continuous. (See, though, Def. 5.2.5 below for a related condition.)

An important feature of the group of translations is that they can be taken arbitrarily small, in which case the translation operator should become (in a suitable sense) arbitrarily close to the identity operator. We can observe how this transpires in terms of the action of translations on (differentiable) wave functions:[33]

$$\lim_{\varepsilon\to 0}(T(\varepsilon)\psi)(x) = \lim_{\varepsilon\to 0}\psi(x-\varepsilon) = \psi(x) - \varepsilon\psi'(x) + O(\varepsilon^2)\ . \tag{5.5}$$

We interpret this result as defining an infinitesimal expansion of the translation operator itself,

$$T(\varepsilon) = 1 - \frac{i\varepsilon}{\hbar}T_{\rm inf} + O(\varepsilon^2)\ , \qquad (T_{\rm inf}\psi)(x) = -i\hbar\psi'(x)\ . \tag{5.6}$$

We have inserted conventional factors of i and $\hbar$ that allows us to make the identification of $T_{\rm inf}$ with the *momentum operator* P.

The relationship between translations and momentum is easier to tease out in momentum space. On generalised momentum eigenstates, we have

$$\begin{aligned}
T(a)\,|p\rangle &= \int_{-\infty}^{\infty} \mathrm{d}x\, T(a)\,|x\rangle\,\langle x|p\rangle &&= \int_{-\infty}^{\infty}\mathrm{d}x\,|x+a\rangle\, e^{\frac{ipx}{\hbar}}\ ,\\
&= \int_{-\infty}^{\infty}\mathrm{d}x\,|x\rangle\, e^{\frac{ip(x-a)}{\hbar}} &&= e^{-\frac{ipa}{\hbar}}\int_{-\infty}^{\infty}\mathrm{d}x\,|x\rangle\, e^{\frac{ipx}{\hbar}}\ ,\\
&= e^{-\frac{ipa}{\hbar}}\,|p\rangle &&= e^{-\frac{iPa}{\hbar}}\,|p\rangle\ ,
\end{aligned} \tag{5.7}$$

so on our (continuum) basis of generalised momentum eigenstates we have the operator relation

$$T(a) = \exp\left(-\frac{iPa}{\hbar}\right)\ , \tag{5.8}$$

from which we formally deduce $T_{inf} = P$ just by taking the power series expansion of the exponential. We summarise this situation by saying that P is the *infinitesimal generator of translations*.[34] Note also that unitarity of $T(a)$ follows from self-adjointness of P and vice versa,

$$T(a)^* = \left(e^{-\frac{iPa}{\hbar}}\right)^* = \left(e^{\frac{iPa}{\hbar}}\right) = T(a)^{-1}\ . \tag{5.9}$$

[33]The restriction to differentiable wave functions here is, once again, related to the infinite dimensionality of our Hilbert space, which means that the infinitesimal version of translation that we are defining is only partially defined on $L^2(\mathbb{R})$. Differentiable wave functions are dense in $L^2(\mathbb{R})$.

[34]If you are familiar with Noether's theorem from classical mechanics, then this should sound familiar as a counterpart of the fact that momentum is the conserved quantity associated with translation invariance, and it generates infinitesimal translations via the Poisson bracket.

Thus far this discussion makes no reference to translations being a *dynamical symmetry* of the system, *i.e.*, being a symmetry of the equations of motion (in our case, the time-dependent Schrödinger equation). Intuitively, this should depend on the potential $V(X)$ being constant (or zero), as otherwise the potential would violate translation invariance. To have translations as a dynamical symmetry, we would like to require that the symmetry transformation of the infinitesimal time evolution of a state vector is the same as the infinitesimal time evolution of the symmetry-transformed state vector, *i.e.*,

$$T(a)\,|H\psi\rangle = H\,|T(a)\psi\rangle \ , \tag{5.10}$$

which, by writing $|\psi\rangle = T(a)^*\,|\phi\rangle$ for some $|\phi\rangle$ we can equivalently characterise as

$$T(a)HT(a)^* = H\,. \tag{5.11}$$

Further looking at the case of infinitesimal translations, this gives the condition

$$\left(1 - \frac{i\varepsilon}{\hbar}P + O(\varepsilon^2)\right) H \left(1 + \frac{i\varepsilon}{\hbar}P + O(\varepsilon^2)\right) = H + \frac{i\varepsilon}{\hbar}[H,P] + O(\varepsilon^2) = H\,, \tag{5.12}$$

from which we deduce the requirement $[H,P] = 0$. Using our expression for finite translations as an exponentiated version of P, one can show that this vanishing commutator also implies the relation (5.11). And indeed, these will hold for a Hamiltonian of the form $H = P^2/2m + V(X)$ only if $V(X)$ is a constant.[35]

5.2 A general theory of quantum symmetries

What we have seen above gives us some insight into the general structure of symmetries in quantum systems. Now we will look at this topic more abstractly.

5.2.1 A first attempt at generalisation

If we try to generalise a bit from what we have seen in our example, we might propose the following structures associated with the presence of a symmetry in a quantum system. It will turn out that these are not quite the complete story; we will return to the correct formulation after some technical discussion.

- Symmetries should be implemented via unitary operators on $\mathcal{H}$, so as to preserve norms and transition amplitudes.
- Symmetries naturally form a group—call it $\mathcal{G}$—and the operators implementing their action on $\mathcal{H}$ should form a unitary representation of that group,

$$U : \mathcal{G} \to \mathsf{U}(\mathcal{H})\,, \qquad U(g_1)U(g_2) = U(g_1g_2) \quad \forall\, g_1, g_2 \in \mathcal{G}\,. \tag{5.13}$$

- For continuous symmetries, infinitesimal transformations are realised by self-adjoint operators that generate finite transformations (parameterised by $s \in \mathbb{R}$) via exponentiation according to

$$U(g(s)) = \exp\left(-\frac{iGs}{\hbar}\right)\,, \quad G = G^*\,. \tag{5.14}$$

- For dynamical symmetries, we require

$$U(g)HU(g^{-1}) = H\,, \qquad ([H,G] = 0 \quad \text{for infinitesimal generators})\,. \tag{5.15}$$

These properties do hold in quite a few examples of interest. For instance, you should compare the above to our discussion of time evolution in Chapter 1. However, they are not the most general version of the story, and we have also been a bit cavalier about some technical details in our discussion of infinitesimal symmetries. We address both of these issues below.

[35] As a concrete example of this, in your first homework exercise, you will have shown that for the harmonic oscillator the finite spatial translation of the ground state is a coherent state, which is certainly no longer an energy eigenstate, let alone the ground state.

5.2.2 Quantum symmetries and projective representations

The main shortcoming of the formulation above arises from having neglected the distinction between Hilbert space $\mathcal{H}$ and the true space of quantum states, $\mathbb{P}(\mathcal{H})$. *A priori*, one expects that a quantum symmetry need only be formulated as a map

$$\mathfrak{s} : \mathbb{P}(\mathcal{H}) \longrightarrow \mathbb{P}(\mathcal{H}) . \tag{5.16}$$

Rather than requiring that overlaps be preserved, it should be sufficient to require that *transition probabilities* are preserved, as these are the physically meaningful quantities. Let us denote a quantum state corresponding to the ray in $\mathcal{H}$ that passes through a vector ψ by $[\psi]$, so $[\psi] = [\lambda\psi]$ for $\lambda \in \mathbb{C}^\times$. For quantum states $[\psi], [\varphi] \in \mathbb{P}(\mathcal{H})$, we then require equality of the transition probabilities:

$$\frac{|\langle\varphi|\psi\rangle|^2}{\|\varphi\|^2\|\psi\|^2} = \frac{|\langle\mathfrak{s}(\varphi)|\mathfrak{s}(\psi)\rangle|^2}{\|\mathfrak{s}(\varphi)\|^2\|\mathfrak{s}(\psi)\|^2} , \tag{5.17}$$

where in this expression, ψ and φ could be any representatives of the quantum states $[\psi]$ and $[\varphi]$, respectively. (The transition probabilities are, as usual, independent of the choice of such representative.) Naively, it appears that this could be a weaker condition than the requirement of a unitary map on $\mathcal{H}$. This is indeed the case, but perhaps to a lesser extent than one might first think. The situation is explained by the following.

Theorem 5.2.1 (Wigner)**.** For any quantum symmetry $\mathfrak{s}$ defined as above on projectivised Hilbert space, there exists an operator $V(\mathfrak{s}) : \mathcal{H} \to \mathcal{H}$ that is compatible with $\mathfrak{s}$ that is either unitary or anti-unitary that induces $\mathfrak{s}$ when treated as a map of rays. When $\dim(\mathcal{H}) \geqslant 2$, the operator $V(\mathfrak{s})$ is unique up to an overall phase.

(In the case that $\dim(\mathcal{H}) = 1$, $V(\mathfrak{s})$ can be chosen to be *either* unitary or anti-unitary for the same $\mathfrak{s}$; in higher dimensional Hilbert spaces it will be one or the other, with no choice involved other than the aforementioned phase.) We will set aside the topic of anti-unitary operators for the moment and focus on symmetries that are realised as unitary operators on $\mathcal{H}$.

Definition 5.2.2. The *projective unitary group* of a Hilbert space $\mathcal{H}$ is the quotient

$$\mathbb{P}\mathsf{U}(\mathcal{H}) = \mathsf{U}(\mathcal{H})/\{e^{i\theta}1_{\mathcal{H}},\ \theta \in \mathbb{R}\}$$

of the group of unitary transformations on $\mathcal{H}$ by the normal subgroup consisting of multiplications by a constant phase.

What Wigner's theorem is telling us, given this definition, is that (neglecting the anti-unitary caveat) a quantum symmetry can be unambiguously lifted to an element of the projective unitary group for the corresponding Hilbert space.

Definition 5.2.3. A *projective unitary representation* of a group $\mathcal{G}$ on a Hilbert space $\mathcal{H}$ is a group homomorphism $U : \mathcal{G} \to \mathbb{P}\mathsf{U}(\mathcal{H})$.

What we should then be interested in are these projective unitary representations of a symmetry group $\mathcal{G}$. We can then lift these symmetries to actual unitary operators, but we have to choose phases. If we do this arbitrarily (choosing arbitrary phases for each $g \in \mathcal{G}$), then at the level of unitary operators the group law may not be obeyed, indeed we only expect

$$U(g_1)U(g_2) = e^{i\xi(g_1,g_2)}U(g_1g_2) , \qquad \xi(g_1,g_2) \in [0,2\pi) . \tag{5.18}$$

Associativity of the multiplication of operators on $\mathcal{G}$ gives a condition on these phases,[36]

$$\xi(g_1,g_2g_3) + \xi(g_2,g_3) = \xi(g_1,g_2) + \xi(g_1g_2,g_3) \mod 2\pi , \tag{5.19}$$

It follows immediately that we have the following

Proposition 5.2.4. A *projective unitary representation* of a group $\mathcal{G}$ on a Hilbert space $\mathcal{H}$ is equivalently a map $U : \mathcal{G} \to \mathsf{U}(\mathcal{H})$ obeying (5.18) and (5.19).

Indeed, this is sometimes used as the definition; physicists will say that "in quantum mechanics, the group law for symmetries only needs to be obeyed up to phase ambiguities". The phase ambiguities in the definitions of the operators

[36] Though it is not important for us, this condition means that the map $\xi : \mathcal{G}\times\mathcal{G} \to U(1)$ is what is known as a *group 2-cocycle valued in* $U(1)$.

$U(g_i)$ themselves means we can modify the phases in (5.18) by taking a map $\phi : \mathcal{G} \to \mathbb{S}^1$ to produce an equivalent projective unitary representation but now with

$$\xi(g_1, g_2) \to \xi(g_1, g_2) + \phi(g_1) + \phi(g_2) \mod 2\pi \,. \tag{5.20}$$

Using this freedom to redefine phases, it turns out that in a large class of examples of continuous groups (when either $\mathcal{H}$ is finite-dimensional or, if infinite-dimensional, if $\mathcal{G}$ is what is called a *semi-simple* group), one can set the phases $\xi(g_1, g_2)$ to be zero for transformations that are suitably close to the identity, thus realising something that looks like a unitary representation for symmetries that are close to the identity. Globally there can be an obstruction to setting these phases to zero for all group multiplications; we will see an explicit example of this in the next chapter in the context of rotations.

5.2.3 One parameter unitary groups

In the discussion of translations some of the statements about the infinitesimal limit may have felt a bit sketchy. There is actually a powerful theorem that puts these statements on firm footing. We start with a definition:

Definition 5.2.5. A *strongly continuous one-parameter unitary group* is a family $U(t)$ for $t \in \mathbb{R}$ of unitary operators on a Hilbert space $\mathcal{H}$ such that

- $U(0) = 1_{\mathcal{H}}$,
- $\forall s, t \in \mathbb{R}\,, \qquad U(t+s) = U(t)U(s)\,,$
- $\forall t \in \mathbb{R}\,, \qquad \lim_{s \to t} U(s)\psi = U(t)\psi\,.$

The first two points defines a one-parameter unitary group, which you will recognise as being the same as a unitary representation of the additive group $(\mathbb{R}, +)$ as we had in the case of translations. The third point is the notion of *strong continuity*. We will not be very attentive to this continuity condition in this course; it will always hold in examples we consider.

Definition 5.2.6. For $U(\cdot)$ a strongly continuous one-parameter unitary group, the *infinitesimal generator* of $U(\cdot)$ is the operator K defined by[37]

$$K\psi = \lim_{t \to 0} \frac{1}{i} \frac{U(t)\psi - \psi}{t} \,. \tag{5.21}$$

It turns out with this definition, K will be defined for a dense subset of $\mathcal{H}$ (or all of $\mathcal{H}$ in the finite-dimensional case). We then have the following:

Theorem 5.2.7 (Stone's Theorem on One-Parameter Unitary Groups)**.** Let $U(\cdot)$ be a strongly continuous, one-parameter unitary group. The infinitesimal generator K of the family is a self-adjoint operator, and for all t we have,

$$U(t) = \exp\left(itK\right) \,. \tag{5.22}$$

Conversely, every self-adjoint operator K generates a strongly continuous one-parameter unitary group this way.

The exponential of K can be defined in terms of its action on a basis of (generalised) K-eigenstates. We will not study a proof of this theorem; instead it is meant to provide a justification for some of the more casual manipulations that have arisen and will arise when studying symmetries in what follows. It should be noted that even in the finite dimensional case this is a non-trivial theorem; it establishes a kind of differentiability for families of operators/matrices based only upon continuity.

We can observe now that the quantity $U(t_1 - t_0)$ that we considered in Chapter 1 and in the discussion of the propagator is precisely a one-parameter unitary group whose infinitesimal generator is the Hamiltonian. This is in the case when the Hamiltonian is time-independent. In the time-dependent case, one actually gets a unitary *groupoid*! We will not discuss this further.

[37] This definition differs by a conventional minus sign and factor of $\hbar$ relative to what we used in the case of momentum and translations. In the quantum mechanical setting we will normally include those additional factors.

5.2.4 Anti-unitary operators

Now we return to the issue of anti-unitary operators, which appeared in the statement of Wigner's theorem, and define such an entity.

Definition 5.2.8. An *anti-unitary* operator on a Hilbert space $\mathcal{H}$ is a surjective linear map $A : \mathcal{H} \to \mathcal{H}$ obeying

$$\langle A\varphi | A\psi \rangle = \overline{\langle \varphi | \psi \rangle} = \langle \psi | \varphi \rangle \ . \tag{5.23}$$

We can see that an anti-unitary operator must be $\mathbb{C}$ anti-linear. A standard example of an anti-unitary operator on a complex Hilbert space is a complex conjugation operation, which takes states of the form

$$\psi = \sum_i c_i \psi_i \quad \longrightarrow \quad A\psi = \sum_i \overline{c_i} \psi_i \ , \tag{5.24}$$

for $\{\psi_i\}$ an orthonormal basis. (This operation clearly depends on the basis.) In the case of $L^2(\mathbb{R})$, one has a similar operation that takes the complex conjugate of a wave function.

An important observation is that if A is anti-unitary, then A^2 is unitary,

$$\left\langle A^2\varphi \middle| A^2\psi \right\rangle = \langle A\psi | A\varphi \rangle = \langle \varphi | \psi \rangle \ . \tag{5.25}$$

This means that any symmetry that can be realised as the square of another symmetry will be realised unitarily on $\mathcal{H}$. In the case of continuous groups of symmetries, like translations and rotations, this lets us get away with ignoring anti-unitary symmetries all together. On a homework exercise, you will investigate the relationship between anti-unitary symmetries and time-reversal.

5.2.5 The form of quantum symmetries

We are now in position to formulate a more precise characterisation of the form that symmetries take in quantum mechanical systems.

- Symmetries are implemented via unitary or anti-unitary operators on $\mathcal{H}$.
- Symmetries naturally form a group, and the operators implementing them form a projective representation of that group on $\mathcal{H}$.
- Continuous symmetries are generated, in the sense of Stone's theorem, by self-adjoint operators via exponentiation.
- For unitarily realised symmetries to be compatible with time evolution (dynamical symmetries), we require any of the following equivalent conditions
  - $U(t)U(g) = U(g)U(t)$,
  - $[H, U(g)] = 0$
  - $[U(t), G] = 0$
  - $[H, G] = 0$

  Here $U(t) = \exp(-iHt/\hbar)$ is the time evolution operator while $U(g)$ is the unitary corresponding to an element $g \in \mathcal{G}$ of the symmetry group. If $U(g)$ is part of a one-parameter group, then its infinitesimal generator is G.