Brief overview of symmetries in quantum mechanics

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If a unitary operator commutes with the Hamiltonian of a quantum system, we say that the Hamiltonian is invariant under the symmetry operation that the unitary operator performs. This is, however, not the only type of symmetry in quantum mechanics. The following table shows the symmetries arising from having a unitary or antiunitary operator commuting or anticommuting with the Hamiltonian [W].

	Unitary operator	Antiunitary operator
Commutes with Hamiltonian	Unitary symmetry	Time reversal symmetry
Anticommutes with Hamiltonian	Chiral symmetry*	Particle-hole symmetry**

* Also sometimes called sublattice symmetry.
** Also sometimes called charge conjugation.

We will make a few comments about these symmetries in the following sections.

1 Unitary symmetry

In general, if a Hamiltonian H is invariant under the symmetry described by the unitary operator $\mathscr{S}$, we have

$$[H,\mathscr{S}]=0 \qquad \Leftrightarrow \qquad H\mathscr{S}-\mathscr{S}H=0 \qquad \Leftrightarrow \qquad \mathscr{S}H\mathscr{S}^\dagger=H. \tag{1}$$

Consider an energy eigenket $|n\rangle$ of H with energy E_n. It follows that

$$H\mathscr{S}|n\rangle=\mathscr{S}H|n\rangle=\mathscr{S}E_n|n\rangle=E_n\mathscr{S}|n\rangle. \tag{2}$$

In other words, $\mathscr{S}|n\rangle$ is also an eigenstate of H with the same energy. There are now two possibilities. Either $|n\rangle$ and $\mathscr{S}|n\rangle$ are distinct quantum states, in

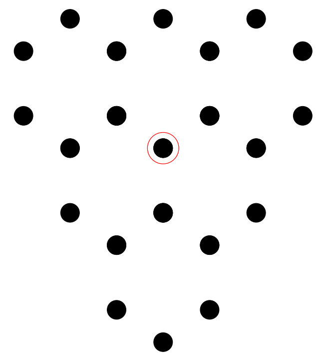

Figure 1: If the honeycomb lattice is rotated by 0, $2\pi/3$, or $4\pi/3$ around the lattice site marked by a red circle, the lattice maps onto itself.

which case there is a degeneracy for energy E_n. Or $|n\rangle$ and $\mathscr{S}|n\rangle$ represent the same quantum state, in which case they at most differ by a global phase, i.e.

$$\mathscr{S}|n\rangle = e^{i\delta}|n\rangle. \tag{3}$$

This equation says that $|n\rangle$ is an eigenket of $\mathscr{S}$. In other words, any nondegenerate energy eigenstate $|n\rangle$ of H is also an eigenstate of $\mathscr{S}$. Note that theorem 6 on page 260 of [SN] is a special case of this theorem.

If two Hermitian matrices H and G commute, they can be diagonalized simultaneously. A unitary operator $\mathscr{S}$ can be written in the form $\mathscr{S} = e^{iG}$, where $G = -i\ln(\mathscr{S})$ is Hermitian, and if G is diagonal, so is e^{iG}. It follows that H and $\mathscr{S}$ can be diagonalized simultaneously, when the unitary operator $\mathscr{S}$ is a symmetry of the Hamiltonian. If we write H as a matrix in the basis of the eigenstates of $\mathscr{S}$ ordered according to eigenvalue of $\mathscr{S}$, H will be block diagonal, where each block corresponds to an eigenvalue of $\mathscr{S}$. As an example, see equation (3.196) in [SN]. This means that the Hamiltonian does not mix different eigenvalues of $\mathscr{S}$, so if the system starts out in an eigenstate of $\mathscr{S}$ with a given eigenvalue, it will continue to be in an eigenstate of $\mathscr{S}$ with the same eigenvalue under time evolution. This is also noted in (4.12) in [SN]. This means that the original problem of diagonalizing the Hamiltonian reduces into diagonalizing several smaller blocks. Each such block is also called a symmetry sector.

Unitary symmetries can be either continuous or discrete. A symmetry is continuous, if one can do an arbitrarily small change. Examples include translations and rotations by an infinitesimal amount. We have already discussed these in chapters 1 and 3 of [SN], so here we will focus on discrete symmetries. Examples of discrete symmetries are lattice translations, lattice rotations, space inversion, mirror planes, and many more. These symmetries are commonly encountered in solid state physics, where various operations can map a crystal lattice onto itself. An example is given in figure 1. We can further divide the discrete symmetries into symmetries with infinitely or finitely many transformations. Lattice translations have infinitely many transformations, since displacement by any vector of the form $\mathbf{R} = n\mathbf{a}_1 + m\mathbf{a}_2 + p\mathbf{a}_3$ will map the lattice onto itself, where n, m, and p are integers and $\mathbf{a}_i$ are the primitive lattice vectors. The other examples given above all have a finite number of transformations. Doing space inversion three times is, for instance, the same as doing space inversion once, so we only have the choices of doing space inversion once or not doing it. Lattice translations give rise to Bloch's theorem and are discussed in detail in the courses on solid state physics, so here we will focus on discrete symmetries with a finite number of transformations. Such symmetries also frequently appear in atomic and molecular physics. In particular, [SN] discusses space inversion as one example, and other discrete symmetries with a finite number of operations can be investigated with similar methods.

2 Chiral symmetry

A Hamiltonian with a chiral symmetry described by a unitary operator Γ fulfils

$$\{H, \Gamma\} = 0 \qquad \Leftrightarrow \qquad H\Gamma + \Gamma H = 0 \qquad \Leftrightarrow \qquad \Gamma H \Gamma^\dagger = -H. \tag{4}$$

Let us first note that

$$\Gamma^2 H \left(\Gamma^\dagger\right)^2 = \Gamma(\Gamma H \Gamma^\dagger)\Gamma^\dagger = -\Gamma H \Gamma^\dagger = H. \tag{5}$$

This means that Γ^2, which is also unitary, is a unitary symmetry of the Hamiltonian. If Γ^2 is not a phase factor times the identity, we can hence write the Hamiltonian in block diagonal form with more than one block.

If Γ^2 is not a phase factor times the identity, we will block diagonalize the Hamiltonian and restrict ourselves to considering only one block. We will continue this process, until we find either no chiral symmetry or find a Γ fulfilling $\Gamma^2 = e^{i\phi}\mathbb{1}$. Note that we can remove the phase by redefining $\Gamma \to \Gamma e^{i\phi/2}$, as $\Gamma e^{i\phi/2}$ is also unitary and anticommutes with the Hamiltonian. We can hence choose Γ such that

$$\Gamma^2 = \mathbb{1}. \tag{6}$$

This means that $\Gamma^{-1} = \Gamma$, and since Γ is unitary, $\Gamma^{-1} = \Gamma^\dagger$, so Γ is also Hermitian. To summarize

$$\Gamma = \Gamma^\dagger = \Gamma^{-1}. \tag{7}$$

If $|n\rangle$ is an energy eigenket of H with energy E_n, then

$$H\Gamma|n\rangle = -\Gamma H|n\rangle = -\Gamma E_n|n\rangle = -E_n\Gamma|n\rangle. \tag{8}$$

This means that $\Gamma|n\rangle$ is an energy eigenket with energy $-E_n$. Since $|n\rangle$ and $\Gamma|n\rangle$ are eigenkets with different energies, they are orthogonal, i.e.

$$\langle n|\Gamma|n\rangle = 0. \tag{9}$$

Furthermore
$$\Gamma(\Gamma|n\rangle) = \Gamma^2|n\rangle = |n\rangle \tag{10}$$
due to (6). In conclusion, the states in the spectrum appear in pairs with energies $\pm E_n$, so the spectrum of the considered block of the Hamiltonian is symmetric around zero energy.

For more information about chiral symmetry see section 1.4 of [TI].

3 Time reversal symmetry

Time reversal symmetry is discussed in detail in section 4.4 of [SN]. Here, we show that an antiunitary operator θ can always be written as $\theta = UK$, where U is a unitary operator and K is complex conjugation. This can be seen as follows. First note that
$$\theta = \theta K^2 = (\theta K)K \tag{11}$$
as K^2 is the identity. It is hence sufficient to show that θK is unitary. In analogy to definition 1 on page 273 of [SN], a transformation $|\alpha\rangle \to U|\alpha\rangle$ and $|\beta\rangle \to U|\beta\rangle$ is said to be unitary if
$$\langle\beta|U^\dagger U|\alpha\rangle = \langle\beta|\alpha\rangle, \tag{12}$$
$$U(c_1|\alpha\rangle + c_2|\beta\rangle) = c_1 U|\alpha\rangle + c_2 U|\beta\rangle. \tag{13}$$
The general kets $|\alpha\rangle$ and $|\beta\rangle$ can be written in terms of the base kets $|n\rangle$ as
$$|\alpha\rangle = \sum_n \alpha_n |n\rangle, \qquad |\beta\rangle = \sum_n \beta_n |n\rangle. \tag{14}$$
Define
$$|\alpha^*\rangle = \sum_n \alpha_n^* |n\rangle, \qquad |\beta^*\rangle = \sum_n \beta_n^* |n\rangle, \tag{15}$$
and
$$|\tilde{\alpha}\rangle = \theta|\alpha\rangle, \qquad |\tilde{\beta}\rangle = \theta|\beta\rangle. \tag{16}$$
Then
$$\theta K|\alpha\rangle = |\tilde{\alpha^*}\rangle, \qquad \theta K|\beta\rangle = |\tilde{\beta^*}\rangle. \tag{17}$$
Since θ is antiunitary, we have
$$\langle\tilde{\beta}|\tilde{\alpha}\rangle = \langle\beta|\alpha\rangle^*, \tag{18}$$
$$\theta(c_1|\alpha\rangle + c_2|\beta\rangle) = c_1^*\theta|\alpha\rangle + c_2^*\theta|\beta\rangle. \tag{19}$$
Note that $|\alpha^*\rangle$ and $|\beta^*\rangle$ are also valid kets, so the above equations are equally valid for $|\alpha^*\rangle$ and $|\beta^*\rangle$. Therefore
$$\langle\tilde{\beta^*}|\tilde{\alpha^*}\rangle = \langle\beta^*|\alpha^*\rangle^* = \left(\sum_n \beta_n \alpha_n^*\right)^* = \sum_n \beta_n^* \alpha_n = \langle\beta|\alpha\rangle, \tag{20}$$

which shows that (12) is fulfilled for $U = \theta K$, and

$$\begin{aligned}\theta K(c_1|\alpha\rangle + c_2|\beta\rangle) = \theta(c_1^*|\alpha^*\rangle + c_2^*|\beta^*\rangle) = c_1\theta|\alpha^*\rangle + c_2\theta|\beta^*\rangle \\ = c_1\theta K|\alpha\rangle + c_2\theta K|\beta\rangle,\end{aligned} \tag{21}$$

which shows that (13) is fulfilled for $U = \theta K$. Hence θK is a unitary operator.

4 Particle-hole symmetry

If a Hamiltonian H has particle-hole symmetry described by the antiunitary operator θ, we have

$$\{H, \theta\} = 0 \qquad \Leftrightarrow \qquad H\theta + \theta H = 0 \qquad \Leftrightarrow \qquad \theta H \theta^{-1} = -H, \tag{22}$$

where $\theta^{-1} = KU^{-1}$ when $\theta = UK$. We first note that

$$\theta^2 H(\theta^{-1})^2 = -\theta H \theta^{-1} = H, \tag{23}$$

so

$$\theta^2 = UKUK = UU^*KK = UU^* \tag{24}$$

is a unitary symmetry. If θ^2 is not proportional to the identity operator, we can hence block diagonalize the Hamiltonian and change focus to a single block. We continue this process until θ^2 is proportional to the identity, or there is no particle-hole symmetry. We cannot remove a phase from θ^2 by letting $\theta \to e^{i\phi}\theta$, as this leads to $\theta^2 \to e^{i\phi}\theta e^{i\phi}\theta = e^{i\phi}e^{-i\phi}\theta^2 = \theta^2$, so generally θ^2 is a phase factor $e^{i\eta}$ times the identity. In fact, the phase factor must be plus or minus one. This is so because $\mathrm{Tr}(\theta^2) = \mathrm{Tr}(UU^*)$ is real. The trace is $\mathrm{Tr}(\theta^2) = De^{i\eta}$, where D is the dimension of the matrix, and hence $e^{i\eta} = \pm 1$.

If $|n\rangle$ is an energy eigenket of H with energy E_n, then

$$H\theta|n\rangle = -\theta H|n\rangle = -\theta E_n|n\rangle = -E_n\theta|n\rangle. \tag{25}$$

In other words, $\theta|n\rangle$ is an eigenstate with energy $-E_n$. The state $\theta^2|n\rangle$ is proportional to $|n\rangle$. The states in the spectrum hence appear in pairs at energies $\pm E_n$, so the spectrum of the considered block is symmetric around zero energy.

References

[W] https://en.wikipedia.org/wiki/Periodic_table_of_topological_insulators_and_topological_superconductors

[SN] J. J. Sakurai and J. Napolitano, Modern Quantum Mechanics, third edition, Cambridge University Press (2021).

[TI] J. K. Asbóth, L. Oroszlány, A. Pályi, A Short Course on Topological Insulators, arXiv:1509.02295.