Applications of Group Representation Theory to Quantum Mechanics

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1 Quantum Mechanics

Quantum mechanics is concerned with solving equations of the form

$$\hat{H}\Psi(\mathbf{x},t) = i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{x},t),$$

where $\hat{H}$ is a Hermitian linear operator known as the Hamiltonian and $\Psi(\mathbf{x},t)$ a vector on a Hilbert space. The previous equation is time-dependent. The corresponding time-independent equation is of the form

$$\hat{H}\psi(\mathbf{x}) = E\psi(\mathbf{x}),$$

where $\hat{H}$ is the same linear operator, E is an eigenvalue of $\hat{H}$ with eigenvector $\psi(\mathbf{x})$.

Definition 1. A **Hilbert space** is a complete metric space and inner product space in which the inner product, denoted as $\langle a, b\rangle$, is complex-valued and obeys the following relations:

(a) $\langle a, b\rangle = \langle b, a\rangle^{\dagger}$

(b) $\langle a + c, b\rangle = \langle a, b\rangle + \langle c, b\rangle$

(c) $\langle a, a\rangle \geq 0$ with equality if and only if a is zero,

where † represents complex conjugation.

In the context of quantum mechanics, Hilbert space vectors describe a system's probability amplitude and are called **state vectors**. Probability amplitude is a complex-valued quantity whose Hilbert space inner product is the probability of measuring the system in a given state. Eigenvectors of Hermitian operators are important because physically measuring a quantum system causes it to be in a state represented by an eigenvector. The quantity measured will be the eigenvalue corresponding to the eigenvector.

Observable quantities in quantum mechanics correspond to Hermitian linear operators $\hat{O}$ on a Hilbert space. To determine the expected value of an observable quantity in a system described by a state vector ψ, one calculates the inner product $\left\langle \psi, \hat{O}\psi \right\rangle$.

Proposition 1. *The eigenvalues of a Hermitian operator are always real and the eigenvectors are always orthogonal.*

A proof derived from Arfken's treatment in *Mathematical Methods for Physicists* can be found on the Wolfram MathWorld website[3]. The Hamiltonian is the operator corresponding to energy. This paper is devoted to determining information about the eigenvalues of a Hamiltonian, known as energy levels, from its symmetries. To this end, we introduce the symmetry group of a Hamiltonian. The symmetry group of a given Hamiltonian is the set of all coordinate transformations and permutations that leave the Hamiltonian invariant. Let T be a symmetry operation. Then,

$$T\hat{H}T^{-1} = \hat{H}$$
$$T\hat{H} = \hat{H}T.$$

This provides our first application of group theory to quantum mechanics.

Proposition 2. *Let E be an energy level of a Hamiltonian $\hat{H}$ and let G be a group of symmetries of $\hat{H}$. Then, elements of G take eigenvectors corresponding to E to eigenvectors corresponding to E.*

Proof. Let T be a symmetry operation in G and let ψ be an eigenvector corresponding to the energy level E.

$$T\hat{H}\psi = TE\psi$$
$$\hat{H}T\psi = ET\psi,$$

implying that $T\psi$ is an eigenvector corresponding to the energy level E. □

Note that this does not provide information about the degeneracy of a given energy level. To obtain that, we must first learn some group representation theory.

2 Representation theory

Loosely speaking, a group representation is a group action on a vector space.

Definition 2. A **group representation** of a group G on a vector space V is a homomorphism from G to the group of linear transformations of V. If the homomorphism is injective, the representation is called **faithful**.

A more intuitive definition is that a group representation is a set of matrices such that their multiplication table obeys the group multiplication table. The table below contains two representations of $\mathbb{Z}_2$, the first two over $\mathbb{C}$ and the third over $\mathbb{C}^2$.

	e	**a**
$\mathbf{\Gamma_0}$	1	1
$\mathbf{\Gamma_1}$	1	-1
$\mathbf{\Gamma_2}$	$\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}$	$\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}$

Table 1: Two representations of $\mathbb{Z}_2$

Note that the representations Γ_0 and Γ_1 appear as part of Γ_2. This can be formalized as follows. We first define the direct sum.

Definition 3. Let V be a vector space and suppose each element of V can be written uniquely as the sum of an element of W and an element of U, where W and U are subsets of V which are disjoint except for the identity vector. Then, V is the **direct sum** of U and V. This is written as

$$V = W \bigoplus U$$

Definition 4. A representation is called **reducible** when it can be expressed as a direct sum of subrepresentations. Equivalently, a representation is reducible if the vector space it is over contains an invariant subspace.

A representation is called **irreducible** if it is not reducible.

Consider the subspace of $\mathbb{C}^2$ consisting of diagonal matrices. Multiplication by either element of Γ_2 takes a diagonal matrix to a diagonal matrix, meaning that Γ_2 is reducible. In particular,

$$\Gamma_2 = \Gamma_0 \bigoplus \Gamma_1.$$

These concepts allow us to prove the following results about representations of the symmetry group of a Hamiltonian.

Theorem 1. *Let $\hat{H}$ be a Hamiltonian and G its symmetry group. Then, the eigenvectors corresponding to an energy level form a basis for a vector space on which G has a representation[1].*

Proof. It was shown in Proposition 2 that symmetries of the Hamiltonian take eigenvectors to eigenvectors corresponding to the same energy level. The vector space generated by all the eigenvectors corresponding to the same energy level is a natural space to represent G on, with a symmetry transformation which takes an eigenvector ψ_1 to an eigenvector ψ_2 being represented in the corresponding way. □

Theorem 2. *If G is the complete symmetry group of some Hamiltonian $\hat{H}$, then the eigenvectors corresponding to an energy level transform irreducibly according to G[1].*

The proof is elementary and can be found in Heine's *Group Theory and Quantum Mechanics* [1].

We will now apply these tools to a simple quantum system. An ammonia (NH_3) molecule spinning about the axis passing through the nitrogen and perpendicular to the triangular hydrogen base has an inversion symmetry; the inter-atom distances remain the same regardless of whether the nitrogen is above or below the rotating base (see Figure 1). The two symmetries must irreducibly transform the possible eigenvectors among themselves, so there must be two eigenvectors. Therefore, there is one doubly degenerate energy state corresponding to this symmetry.

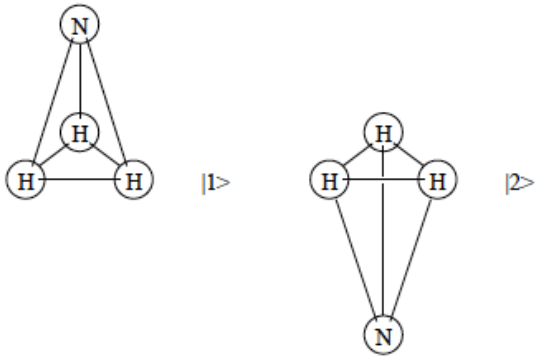

Figure 1: Two states of the ammonia molecule. Image adapted from Daniel Styer's *The Physics of Quantum Mechanics*[2].

3 Perturbation theory

It is an unfortunate fact that the Hamiltonian of almost any system more complicated than the hydrogen atom gives rise to an analytically unsolvable partial differential equation. A great deal

of quantum mechanics is done using various approximation techniques. Perturbation theory is a technique which is useful in systems which would be solvable if not for some relatively small portion of the Hamiltonian. It historically arose as a technique for studying the effect of planets on each others' solar orbits. Solving that problem analytically would require an analytical solution to the three-body problem. Instead, one first solves for the orbits of the planets around the sun, then perturbs those solutions with an interaction term.

The full Hamiltonian is written in the form

$$\hat{H} = \hat{H}_0 + \hat{H}_1,$$

the system

$$\hat{H}_0\psi = E\psi$$

is solved analytically, and approximate energies and state vectors for $\hat{H}_1$ are built from the eigenvectors and energies for $\hat{H}_0$. The building up of new solutions involves evaluating many inner products, which on an infinite dimensional function space amounts to evaluating integrals. Group representation theory can simplify this problem by determining how many originally degenerate energy levels will be split into distinct energy levels and which inner products will evaluate to zero. We will not state a theorem for the second of those uses, as it requires a deeper knowledge of representation theory. A proof of the following theorem can be found in Heine's *Group Theory and Quantum Mechanics*[1].

Theorem 3. *If G is a symmetry group for $\hat{H}, \hat{H}_0$, and $\hat{H}_1$, and if the eigenvectors corresponding to some energy level of $\hat{H}_0$ transform according to the representation Γ of G, where*

$$\Gamma = \Gamma_1 \bigoplus \Gamma_2 \bigoplus \dots \bigoplus \Gamma_n$$

and each Γ_i is irreducible, then the unperturbed energy level is split into at most n levels.

To make sense of this theorem, recall that eigenvectors corresponding to the same energy level transform irreducibly by Theorem 2. Each irreducible subrepresentation Γ_i corresponds to a set of eigenvectors which it sends to each other and which therefore are in the same energy level. Since Γ_i is part of the representation of a symmetry group of the perturbing Hamiltonian, these sets of eigenvectors must be part of the same energy level of the full Hamiltonian, so there can be no more energy levels than there are irreducible subrepresentations.

Returning to the example of the ammonia molecule, suppose we apply a uniform electric field along the axis passing through the nitrogen. The original eigenvectors, corresponding to the nitrogen atom being above or below the hydrogen plane, can be parametrized as being at the points $(0, 1)$ and $(0, -1)$. The only symmetry shared by the original and perturbing Hamiltonians is the identity. In our parametrization, this symmetry would be represented by I_2, the two-dimensional identity matrix. This contains the two one-dimensional identity subrepresentations, so the formerly doubly-degenerate energy level is split into two non-degenerate energy levels.

4 Summary

Group representation theory can be used as a framework for computing values in quantum mechanics. For applications less trivial than the two-state system we have used as an example, it is necessary to have a deeper understanding of group representation theory, particularly the intricacies of representing infinite groups, decomposition of direct products of representations into direct sums of representations, and some theorems on characters of representations.

References

[1] Volker Heine. *Group Theory in Quantum Mechanics*, volume 9 of *Pure and Applied Mathematics*. Pergamon Press Limited, Bristol, first edition, 1960.

[2] Daniel Styer. *The Physics of Quantum Mechanics*. August 2011.

[3] Eric Weisstein. Hermitian operator. http://mathworld.wolfram.com/HermitianOperator.html, 2012.