Wigner's Symmetry Representation Theorem

At the Heart of Quantum Field Theory!

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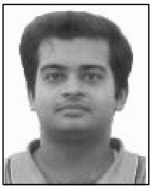

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This article elucidates the important role the notion of symmetry has played in physics. It discusses the proof of one of the important theorems of quantum mechanics, viz., Wigner's Symmetry Representation Theorem. It also shows how the representations of various continuous and discrete symmetries follow from the theorem and at last provides an explicit form of the anti-unitary time-reversal operator.

1. Introduction

A symmetry transformation is a change in our point of view that does not alter the results of possible experiments. Symmetry and invariance have played a very important role in our understanding of physical systems for long and physicists have always relied on this beautiful tool to extract important consequences about the systems under their consideration. For example, the invariance of the laws of physics with respect to translations of both space and time was an assumption which guided the early physicists although any sophisticated formulation for this came much later. The notion of Galilean invariance, which says that the laws of physics will remain the same for two observers who are moving with some uniform relative velocity between themselves, was also embodied in the Newton's laws of motion. However, the principle of symmetry was not held as something very fundamental. Instead, the conservation laws, especially that of momentum and energy, were treated as more sacrosanct. These conservation laws were regarded as the consequences of the laws of motion rather than as

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manifestations of the symmetries underlying these laws of motions.

It was only in the beginning of the twentieth century when people understood that the symmetry of a system is more fundamental and dictates the form of the dynamical laws. Owing to the monumental studies of Lorentz, Poincaré and Einstein, it was established that the Maxwell's laws of electrodynamics embodies a symmetry principle called Lorentz invariance (invariance of physical laws under boosts and rotation). In 1915, Einstein showed that the dynamics of gravity followed from the Equivalence Principle which was in fact a principle of local symmetry: the laws of physics are invariant under local changes of space–time coordinates. However, it was Emmy Noether who through a beautiful theorem published in 1918 explicitly showed that conservation laws were in fact manifestations of the symmetries of the system and there exists a conserved quantity for any continuous symmetry present in the system.

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Quantum mechanics was born shortly later in the 1920s and obviously a natural question was how to incorporate the principles of symmetry into this new framework. It was Eugene Wigner who, in 1931, precisely defined what symmetry meant in this context and explained how a symmetry transformation could be represented by either a unitary or an anti-unitary operator in the Hilbert space of states. Apart from this important theorem, he also published a series of papers on atomic structure and molecular spectra (later published as a book), worked out the representations of the rotation group in three dimensions and laid the foundation for the application of group theory in quantum mechanics. In this article we will, however, restrict ourselves to Wigner's symmetry representation theorem.

In quantum scenario, we define symmetry transformations as those transformations which preserve transition probabilities between the states.

2. Symmetry in Quantum Mechanics

As said earlier, a symmetry transformation is a change in our point of view of looking at a system that does not alter the results of possible experiments. In quantum mechanics, we know that (pure) states are denoted by wave functions in the Hilbert space and the measurable quantities are not the wave functions themselves but the expectation values of any observable quantity. The probability of obtaining an expectation value after measurement depends on the transition probabilities between states which is given by the square of the modulus of the overlap of two wave functions. Hence, a symmetry transform should keep these probabilities invariant. So, in quantum scenario, we define symmetry transformations as those transformations which preserve transition probabilities between the states.

Mathematically, however, physical states are denoted by 'rays' in the Hilbert space. A set of normalized states whose elements differ only by a complex phase are called rays, i.e., the states ψ and $e^{i\theta}\psi$ both belong to the same ray $\mathbb{R}$ for some real θ and denote the same physical state. Hence, a symmetry transformation is a ray transformation T such that if $T : \mathbb{R}_1 \longrightarrow T\mathbb{R}_1$ and $T : \mathbb{R}_2 \longrightarrow T\mathbb{R}_2$, then

$$|\langle\psi_1'|\psi_2'\rangle|^2 = |\langle\psi_1|\psi_2\rangle|^2 \tag{1}$$

for any $\psi_1\epsilon\mathbb{R}_1,\ \psi_2\epsilon\mathbb{R}_2$ and $\psi_1'\epsilon T\mathbb{R}_1,\ \psi_2'\epsilon T\mathbb{R}_2$. That was about the transition probabilities, but how do the individual states themselves transform under a symmetry transformation? The answer to this particular question was provided by Wigner.

3. The Theorem and its Proof

The theorem given by Wigner in 1931, which is a cornerstone of the mathematical formulation of quantum mechanics, states that:

"Any symmetry transformation can be represented on the Hilbert space of physical states by an operator that is either linear and unitary or anti-linear and anti-unitary."

The theorem was stated and first proved by Wigner himself in his book *Group theory and its application to the quantum mechanics of atomic spectra* in the year 1931 [1]. Thereafter it has been proved by many till date, most prominent being those by Bargmann, Ulhorn and Weinberg. Here, we discuss the proof given by Weinberg step-by-step stressing the necessity of each step in details, with certain comments and modifications [2]. The proof stands on the sole principle which we discussed in the previous section: 'conservation of transition probabilities'.

Step 1: An orthonormal and complete set of basis vectors remains so after symmetry transformation.

Let $\{\psi_k \epsilon \mathbb{R}_k\}_{k=1}^n$ be a complete orthonormal basis. Then,

$$|\langle\psi_k|\psi_l\rangle| = \delta_{kl}\,. \tag{2}$$

Let ψ'_k be some arbitrary choice of vector belonging to the transformed ray $\mathbb{R}_k$. Then, we have

$$|\langle\psi'_k|\psi'_l\rangle|^2 = |\langle\psi_k|\psi_l\rangle|^2 = \delta_{kl}\,. \tag{3}$$

But $|\langle\psi'_k|\psi'_k\rangle|$ is real and positive. Hence $|\langle\psi'_k|\psi'_k\rangle| = 1$. Therefore,

$$|\langle\psi'_k|\psi'_l\rangle| = \delta_{kl}\,. \tag{4}$$

This shows that orthonormality is preserved in a symmetry transformation. Again, let $\{\psi'_k\}_{k=1}^n$ be non-complete. Then, $\exists\Psi' \epsilon T\mathbb{R}$ such that

$$|\langle\Psi'|\psi'_k\rangle| = 0 \quad \text{for all } k. \tag{5}$$

Therefore, $|\langle\Psi|\psi_k\rangle|^2 = |\langle\Psi'|\psi'_k\rangle|^2 = 0$ for all k, which is impossible since $\{\psi_k\}_{i=i}^n$ is a complete set. So our hypothesis was wrong and hence completeness is also preserved in a symmetry transformation.

Step 2: Constructing a bijective map on the Hilbert space.

Since the theorem tells that we can represent a symmetry transformation on the Hilbert space by a unitary or anti-unitary operator, we will try to construct a map and show that it represents a symmetry transformation. Let us construct a state $\phi_k = \frac{1}{\sqrt{2}}(\psi_1 + \psi_k)\ \epsilon\, \xi_k,\ (k \neq 1)$. Any state vector ϕ'_k in the transformed ray $T\xi_k$ can be written as a linear combination of the basis elements since we have already shown that the transformed basis elements also form a complete and orthonormal set.

$$\phi'_k = \sum_l c_{kl}\psi'_l\,. \tag{6}$$

Now, invariance of $|\langle\psi_1|\phi_k\rangle|^2$ and $|\langle\psi_k|\phi_k\rangle|^2$ yields

$$|c_{k1}| = \frac{1}{\sqrt{2}}, \quad |c_{kk}| = \frac{1}{\sqrt{2}}, \quad |c_{kl}| = 0, \text{for } l \neq k, 1\,. \tag{7}$$

Choose $c_{k1} = c_{kk} = \frac{1}{\sqrt{2}}$ and $c_{kl} = 0$ for $l \neq k, 1$ and call this transformation U. Hence,

$$U\phi_k = U[\frac{1}{\sqrt{2}}(\psi_1 + \psi_k)] = \frac{1}{\sqrt{2}}[U\psi_1 + U\psi_k]\,. \tag{8}$$

So we have constructed a map and defined its action on a particular state. But, that is not enough! We have to know its action on the entire Hilbert space. So, let us proceed in that direction.

Step 3: Action of the map on a general state vector.

Consider the state $\psi = \sum_k c_k\psi_k$. Again, we use the completeness of $\{U\psi_k\}_{k=1}^{k=n}$ and write the transformed state as

$$\psi' = \sum_k c'_k U\psi_k\,. \tag{9}$$

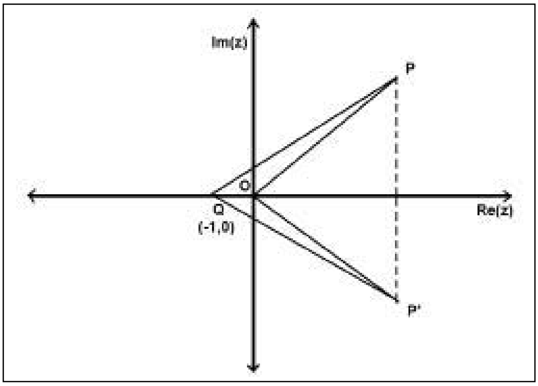

Figure 1. The two possible solutions of the transformed state.

From the invariance of $|\langle\psi_k|\psi\rangle|^2$ and $|\langle\phi_k|\psi\rangle|^2$, one obtains two conditions

$$|c_k|^2 = |c_k'|^2 \quad \forall k \tag{10}$$
$$|c_k + c_1|^2 = |c_k' + c_1'|^2 \quad \forall k \neq 1\,. \tag{11}$$

Dividing (10) and (11) by $|c_1^2|$, one has $|\frac{c_k}{c_1}|^2 = |\frac{c_k'}{c_1'}|^2$ and $|1 + \frac{c_k}{c_1}|^2 = |1 + \frac{c_k'}{c_1'}|^2$. Weinberg solves these two equations algebraically, but they can also be visualised graphically as in *Figure* 1. The points P and P' denote $\frac{c_k}{c_1}$ and $\frac{c_k^*}{c_1^*}$, respectively. The last two expressions impose the constraint that both $|OP|$ and $|QP|$ should remain invariant. Then, this has only two solutions, either P remains at P or goes to P$'$, that is,

$$\mathrm{Re}\left(\frac{c_k'}{c_1'}\right) = \mathrm{Re}\left(\frac{c_k}{c_1}\right), \tag{12}$$
$$\mathrm{Im}\left(\frac{c_k'}{c_1'}\right) = \pm\mathrm{Im}\left(\frac{c_k}{c_1}\right). \tag{13}$$

Hence, either $\frac{c_k'}{c_1'} = \frac{c_k}{c_1}$ or $\frac{c_k'}{c_1'} = \frac{c_k^*}{c_1^*}$.

But, what if $|c_1| = 0$? In that case, we will define our ϕ_k as $\frac{1}{\sqrt{2}}(\psi_i + \psi_k)$ such that $\psi_i \neq 0$ and $\psi_1 \neq \psi_1$ and then we can continue with the proof. This can be done since for any non-trivial vector Ψ, we can at least find one of the $|c_k| \neq 0$.

Step 4: To show that only one of the two relations will hold for all '*k*'.

The last step showed that for a given general state, each of the coefficients has two choices of transformation. Next, we would show that different coefficients of a state cannot transform differently according to the choices but all of them must follow the same choice. To show this, we assume that two distinct coefficients transform differently. Let the complex ratios $\frac{c'_k}{c'_1} = \frac{c_k}{c_1}$ and $\frac{c'_l}{c'_1} = \frac{c^*_l}{c^*_1}$ for $l \neq k$ and $l \neq k \neq 1$. Then, define

$$\Phi = \frac{1}{\sqrt{3}}(\psi_1 + \psi_k + \psi_l)\,. \tag{14}$$

Then the transformed state will be $\Phi = \frac{1}{\sqrt{3}}(U\psi_1 + U\psi_k + U\psi_l)$ by following the same argument as in step 2. Invariance of $|\langle\Phi|\psi\rangle|^2$ and corresponding division by $|c_1|^2$ on both sides with a slight algebraic manipulation will yield

$$\mathrm{Im}(\frac{c_k}{c_1})\mathrm{Im}(\frac{c_l}{c_1}) = 0\,, \tag{15}$$

which is a contradiction since we started out with complex ratios.

Depending on which of the alternatives are realised, define $U\psi$ to be the particular one of the ψ's belonging to the ray $T\mathbb{R}$ such that either $c'_1 = c_1$ or $c'_1 = c^*_1$, respectively. Then,

$$\text{either} \quad U\psi = U\sum_k c_k\psi_k = \sum_k c_k U\psi_k \tag{16}$$

$$\text{or} \quad U\psi = U\sum_k c_k\psi_k = \sum_k c^*_k U\psi_k\,. \tag{17}$$

But what if a state vector Ψ_1 transforms according to (16) and another state Ψ_2 transforms according to (17)? We will show that this cannot happen.

Step 5: To show that the same choice applies to all the state vectors.

Let $\Psi_A = \sum_k a_k\psi_k$ transform according to (16) and $\Psi_B = \sum_k b_k\psi_k$ transform according to (17). Then, invariance of $|\langle\Psi_A|\Psi_B\rangle|^2$ will lead to

$$|\sum_k a_k^* b_k|^2 = |\sum_k a_k b_k|\,. \tag{18}$$

Expanding this and just arranging the indices lead to

$$\sum_{k,l} \mathrm{Im}(a_k^* a_l)\mathrm{Im}(b_k^* b_l) = 0\,. \tag{19}$$

Then, one can always find a third state Ψ_C so that

$$\sum_{k,l} \mathrm{Im}(c_k^* c_l)\mathrm{Im}(a_k^* a_l) \neq 0\,, \tag{20}$$

$$\sum_{k,l} \mathrm{Im}(c_k^* c_l)\mathrm{Im}(b_k^* b_l) \neq 0\,. \tag{21}$$

This can be achieved by the following prescription.

1 Find some (k,l) so that $a_k^* a_l$ and $b_k^* b_l$ are complex, then choose all $c_i = 0$ except c_k and c_l and choose these two coefficients to have different phases.

2 If $a_k^* a_l \neq 0$ but $b_k^* b_l = 0$, then choose a (m, n) such that $b_m^* b_n \neq 0$. If $a_m^* a_n$ is complex, then proceed as Step 1 with c_m and c_n having different phases. If $a_m^* a_n$ is real, then choose c_m, c_n, c_k and c_l with all different phases.

3 If $a_k^* a_l = 0$ but $b_k^* b_l \neq 0$ proceed in the same way as the previous one.

Then, $\sum_{k,l} \mathrm{Im}(c_k^* c_l)\mathrm{Im}(a_k^* a_l) \neq 0 \implies$ same choice between (16) and (17) must be made for Ψ_A and Ψ_C.

$\sum_{k,l}\mathrm{Im}(c_k^* c_l)\mathrm{Im}(b_k^* b_l) \neq 0 \Longrightarrow$ same choice between (16) and (17) must be made for Ψ_B and Ψ_C. This implies that same choice between (16) and (17) must also be made for Ψ_A and Ψ_B, with which we started. So for a given symmetry transformation, all the state vectors must transform according to (16) or (17).

Step 6: To show that the transformation is unitary (or anti-unitary) and linear (or anti-linear).

If Ψ_A and Ψ_B transform according to (16), then

$$\begin{aligned} U(\alpha\Psi_A + \beta\Psi_B) &= U\sum_k(\alpha a_k + \beta b_k)\psi_k \\ &= \alpha\sum_k a_k U\psi_k + \beta\sum_k b_k U\psi_k \\ &= \alpha U\Psi_A + \beta U\Psi_B \qquad (22) \\ \langle U\Psi_A | U\Psi_B\rangle &= \langle\sum_k a_k^* U\psi_k | \sum_k b_k U\psi_k\rangle \\ &= \sum_k a_k^* b_k \\ &= \langle\Psi_A|\Psi_B\rangle \qquad (23) \end{aligned}$$

$\Longrightarrow$ **unitary and linear transformation.**

If Ψ_A and Ψ_B transform according to (17), then

$$\begin{aligned} U(\alpha\Psi_A + \beta\Psi_B) &= U\sum_k(\alpha a_k + \beta b_k)\psi_k \\ &= \alpha^*\sum_k a_k^* U\psi_k + \beta^*\sum_k b_k^* U\psi_k \\ &= \alpha^* U\Psi_A + \beta^* U\Psi_B \qquad (24) \\ \langle U\Psi_A | U\Psi_B\rangle &= \langle\sum_k a_k U\psi_k | \sum_k b_k^* U\psi_k\rangle \\ &= \sum_k a_k b_k^* \\ &= \langle\Psi_A|\Psi_B\rangle^* \qquad (25) \end{aligned}$$

$\Longrightarrow$ **anti-unitary and anti-linear transformation.**

So, this proves the theorem. But, now for any system, there can be numerous symmetries. So, how do we know which symmetry can be represented by unitary operator and which of them by anti-unitary operators on the Hilbert space?

4. Representation of Continuous Symmetry

Continuous symmetries are characterised by invariance following a continuous change in some parameters of the system.

Continuous symmetries are characterised by invariance following a continuous change in some parameters of the system. Space–time symmetries such as rotation, boost (together forms proper orthochronous Lorentz transformation) and translation belong to this class. In case of a rotationally symmetric system, one can rotate the system about an axis continuously through different angles keeping the laws of physics invariant. Similarly for boost and translation, the parameters are rapidity and distance, respectively. It can be shown that continuous symmetry transformations are represented by unitary operators. Since these symmetries have a group structure, any continuous transformation can be written as a composition of two continuous transformations. Hence, if T be such a symmetry, then one has that:

$$T(a) = T(b)T(c) \ , \tag{26}$$

where *a, b and c* are some parameters of the transformation (such as angle, rapidity or distance). If U be a representation of T on Hilbert space, then one also has

$$U(a) = U(b)U(c)e^{i\theta} \, , \tag{27}$$

where θ is any real number. This extra phase factor on the right-hand side (RHS) can be avoided if one considers the representation of T on the ray space instead of the Hilbert space, but this does not in any way affect the following argument. Wigner's theorem says that U can be *either* unitary *or* anti-unitary. Now, the RHS is unitary since the product of two unitary or two anti-unitary operators is always unitary as also is the pure

Continuous symmetries have unitary representations.

phase factor. So, U must be unitary to satisfy the equation. It follows hence that the continuous symmetries have unitary representations.

5. Representation of Discrete Symmetry

These types of symmetries are characterised by invariance following a non-continuous change in the system. Space–time symmetries such as time reversal (T) and parity (P), which together form improper Lorentz transformation, belong to this class. Let us try to determine the nature of these transformations following the method given in the last section. For these symmetry transformations, one has

$$P^{-1} = P \quad \text{so} \quad P^2 = \mathbb{I} \tag{28}$$

$$T^{-1} = T \quad \text{so} \quad T^2 = \mathbb{I} \tag{29}$$

Since the RHS $\mathbb{I}$ is unitary, P and T can be either unitary or anti-unitary. We cannot definitely say which one is the correct representation since both the choices satisfy the last equation. So, we need some other way to determine their nature.

Let us consider the effect of proper orthochronous Lorentz transformation (rotation and boost) Λ on the states in the Hilbert space. Equivalently, we can also look at the passive transformation of the energy-momentum operator P^μ. Since the representation of this transformation is unitary (as discussed in the last section), $U(\Lambda)$ denotes a unitary representation of Λ and we have

$$U(\Lambda)^{-1} P^\mu U(\Lambda) = \Lambda^\mu_\nu P^\nu, \tag{30}$$

So similarly for parity and time reversal, we expect that

$$P^{-1} P^\mu P = \mathcal{P}^\mu_\nu P^\nu, \tag{31}$$

$$T^{-1} P^\mu T = \mathcal{T}^\mu_\nu P^\nu, \tag{32}$$

where the parity and time reversal matrix elements are given by

$$\mathcal{P} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} \text{and}$$

$$\mathcal{T} = \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

Considering the $\mu = 0$ component and noting that the time component of the energy–momentum operator is the Hamiltonian H, one has

$$P^{-1}HP = H, \quad (33)$$

$$T^{-1}HT = -H\,. \quad (34)$$

The first one says that the Hamiltonian is invariant under parity. So parity symmetry can be represented by unitary operators. But the second one says that the Hamiltonian is invariant under time reversal if and only if $H = -H$ or H = 0, which is absurd! So where did we falter? To resolve this let us look at the origin of (30). The space translation operator $T(a) = \exp(-iP.a)$ transforms under Lorentz transform as

$$U(\Lambda)^{-1}T(a)U(\Lambda) = T(\Lambda^{-1}a)\,, \quad (35)$$

For infinitesimal a^μ we have

$$U(\Lambda)^{-1}(\mathbb{I} - ia_\mu P^\mu)U(\Lambda) = \mathbb{I} - i(\Lambda^{-1})_\nu{}^\mu a_\mu P^\nu \quad (36)$$

$$= \mathbb{I} - i(\Lambda)^\mu{}_\nu a_\mu P^\nu\,. \quad (37)$$

So, for the special case of time reversal this becomes

$$T^{-1}(\mathbb{I} - ia_\mu P^\mu)T = \mathbb{I} - i(\mathcal{T})^\mu{}_\nu a_\mu P^\nu\,. \quad (38)$$

Time-reversal symmetry transformations are represented by anti-unitary operators on the Hilbert space.

Identifying the coefficients of $-ia^\mu$ on both sides we get the previous absurd condition! To remedy this we need to apply the anti-unitary condition:

$$T^{-1} i T = -i \tag{39}$$

which yields

$$T^{-1} P^\mu T = -\mathcal{T}^\mu{}_\nu P^\nu . \tag{40}$$

Identifying the $\mu = 0$ component on both sides, $T^{-1}HT = H$, the correct expression for time-reversal invariance. Hence, time-reversal symmetry transformations are represented by anti-unitary operators on the Hilbert space. The purpose of the next section is to provide an explicit form of the time-reversal operator.

6. Time-Reversal Operator

We start by considering the physical implication of the notion of time-reversed Hamiltonian. If $q(t)$ and $p(t)$ are the solutions of the Hamilton's equations of motion,

$$\dot{q} = \frac{\partial H}{\partial p} = \{q, H\} \qquad \dot{p} = -\frac{\partial H}{\partial q} = \{p, H\} , \tag{41}$$

then it is evident that $q(-t)$ and $-p(-t)$ are the solutions of the modified Hamiltonian *H(q,-p)*. Since $q(-t)$ and $-p(-t)$ are the corresponding *time-reversed solution* of $q(t)$ and $p(t)$, we can say that the operation on the Hamiltonian which produces this solution is the time-reversal operation. So, the action of this operator is to transform the Hamiltonian by reversing the direction of the momenta. Since the classical to quantum correspondence is given by simply the Poisson bracket-commutator correspondence, even in the quantum case, one expects that time-reversal operator transforms the Hamiltonian by reversing the direction of all the momenta. But, there is a slight difference in this case since we have the spin angular momenta in addition to the linear momenta operator. Both of them will change sign under time-reversal. Hence, the Hamiltonian transforms as $H \longrightarrow H'$ such that

$$H'(\mathbf{r}, \mathbf{p}, \mathbf{s}) = H(\mathbf{r},\text{-}\mathbf{p},\text{-}\mathbf{s})\,, \qquad (42)$$

where $\mathbf{r}$, $\mathbf{p}$ and $\mathbf{s}$ are the position, linear momenta, and spin angular momenta respectively. Our next step will be to find the explicit form of the operator K doing this transformation such that:

$$KH(\mathbf{r},\mathbf{p},\mathbf{s})K^{-1} = H' = H(\mathbf{r},\text{-}\mathbf{p},\text{-}\mathbf{s})\,. \qquad (43)$$

But for that, we need to consider how the general wave function and Hamiltonian for a n-electron system can be written.

6.1 *General Wave Function and Hamiltonian for n-Electron System*

For a single electron one can write the wave function as a two-component object consisting of spatial and spin part. The spin projections can be just in two directions since we are dealing with a spin-half object, so the wave function will be

$$\psi(\mathbf{r}, s) = \phi_{(\frac{1}{2})}(\mathbf{r})\xi^{(\frac{1}{2})} + \phi_{(-\frac{1}{2})}(\mathbf{r})\xi^{(-\frac{1}{2})} = \sum_{s=\pm\frac{1}{2}} \phi_s(\mathbf{r})\xi^s\,, \qquad (44)$$

where $\phi_s(\mathbf{r})$ is the spatial part and ξ^s denotes the unit vector in 2-D spin space. Now, the Pauli matrices have the property that any 2D matrix can be written as a linear combination of the Pauli matrices and the identity. In addition, if the matrix is hermitian, then the coefficients of the linear combinations will be real. We use this property to express the Hamiltonian, which is a hermitian operator, in terms of the identity and the Pauli matrices.

$$H(\mathbf{r},\mathbf{p},\mathbf{s}) = H_0(\mathbf{r},\mathbf{p})\mathbb{I} + H_x(\mathbf{r},\mathbf{p})s_x + H_y(\mathbf{r},\mathbf{p})s_y + H_z(\mathbf{r},\mathbf{p})s_z\,, \qquad (45)$$

where H_0 and H_x are the operators, which act only on the spatial part and s_x, s_y and s_z are the Pauli matrices. So extending this to an n-electron system, the wave function will be

$$\psi(\mathbf{r}_1, \cdots, \mathbf{r}_n, s_1, \cdots, s_n) = \sum_{all\ \ s_i=\pm\frac{1}{2}} \phi_{s_1 \cdots s_n}(\mathbf{r}) \xi^{s_1} \cdots \xi^{s_n} \,. \tag{46}$$

For an n-electron system, therefore, the Hamiltonian can be written in the following form

$$H(\mathbf{r}_1, \cdots, \mathbf{r}_n, \mathbf{p}_1, \cdots, \mathbf{p}_n, \mathbf{s}_1, \cdots, \mathbf{s}_n) = H^0 + H^1 + H^2 + \cdots \,, \tag{47}$$

where

$$H^0 = H^0(\mathbf{r}, \mathbf{p}) \prod_{i=1}^{i=n} \mathbb{I}_i \,, \tag{48}$$

$$H^1 = \sum_{i=1}^{n} (H_{x_i} s_{x_i} + H_{y_i} s_{y_i} + H_{z_i} s_{z_i}) \prod_{j \neq i} \mathbb{I}_j \,, \tag{49}$$

$$H^2 = \sum_{i \neq j} (H_{x_i x_j} s_{x_i} s_{x_j} + H_{x_i y_j} s_{x_i} s_{y_j} + \cdots) \times \prod_{k \neq i,j} \mathbb{I}_k \,, \tag{50}$$

i and j being the particle indices [4]. It is worthwhile to note that each of these terms in the Hamiltonian is a direct product of n terms corresponding to the operators for each of the n electrons. Still, we can attempt to understand what each term signifies. H^0 will contain operators such as kinetic energy, background potential and inter-electronic potential which depend solely on the position and momentum. The second term will represent the spin–orbit couplings. The rest of the terms will represent higher order couplings in general.

6.2 *Constructing the Time-Reversal Operator*

We can show that in the single electron case, the time-reversal operator is:

$$K = is_y C\,, \tag{51}$$

where C is the complex conjugation operator defined as $C\phi(\mathbf{r}) = \phi^*(\mathbf{r})$ [4]. Since $(CHC^{-1})\phi = CH\phi^* = H^*\phi$, so one has

$$CHC^{-1} = H^*\,. \tag{52}$$

From the form of the Hamiltonian (45), it is clear that complex conjugation affects only through $\mathbf{p} = -i\hbar\nabla$ and s_y, because these are the the only two places with complex elements. So,

$$CHC^{-1} = H_0(\mathbf{r},\text{-}\mathbf{p})\mathbb{I} + H_x(\mathbf{r},\text{-}\mathbf{p})s_x - H_y(\mathbf{r},\text{-}\mathbf{p})s_y + H_z(\mathbf{r},\text{-}\mathbf{p})s_z\,. \tag{53}$$

Then by direct calculation, one has

$$\begin{aligned} KHK^{-1} &= (is_y)CHC^{-1}(is_y)^{-1} \\ &= H_0(\mathbf{r},\text{-}\mathbf{p})\mathbb{I} - H_x(\mathbf{r},\text{-}\mathbf{p})s_x - H_y(\mathbf{r},\text{-}\mathbf{p})s_y \\ &\quad -H_z(\mathbf{r},\text{-}\mathbf{p})s_z \\ &= H(\mathbf{r},-\mathbf{p},-\mathbf{s})\,. \end{aligned}$$

The LHS is what we called the time-reversed Hamiltonian in the previous subsection. So indeed the operator K transforms the Hamiltonian to its time-reversed counterpart and hence it is the time-reversal operator. For an n-electron system, it can be shown similarly that the corresponding operator is

$$K = i^n s_{y_1} s_{y_2} \ldots s_{y_n} C\,. \tag{54}$$

It can be easily verified that the time-reversal operator constructed in this way is anti-unitary as discussed previously. The fact that that the time-reversal symmetry can be represented by an anti-unitary operator has interesting consequences. One such consequence is the Kramer's Degeneracy Theorem which says that "the energy levels of a system with an odd number of electrons remain at least doubly degenerate in the absence of any magnetic field". It was Wigner who first proved this theorem in 1932 and he pointed out that this degeneracy is a manifestation of time-reversal symmetry. But, the theorem is more general in the sense that it holds for any system with an odd number of fermions having a symmetry which is represented by an anti-unitary operator. So, the symmetry under time reversal is just a special case of a more general scenario. A beautiful discussion of the theorem can be found in M J Klein's article [4].

7. Conclusion

Symmetry principles play a powerful role in determining the properties of various systems. Hence, it has been the tool for particle physicists, to understand the physics of various particles and their interactions. The credit for this goes to geniuses, like Wigner, who were the first to understand the importance of symmetry in physics. In the words of another great physicist David J Gross [5], "If we have gone so far in our understanding of symmetry in this century, it is in large part by standing on the shoulders of giants such as Eugene P Wigner."

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Suggested Reading

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