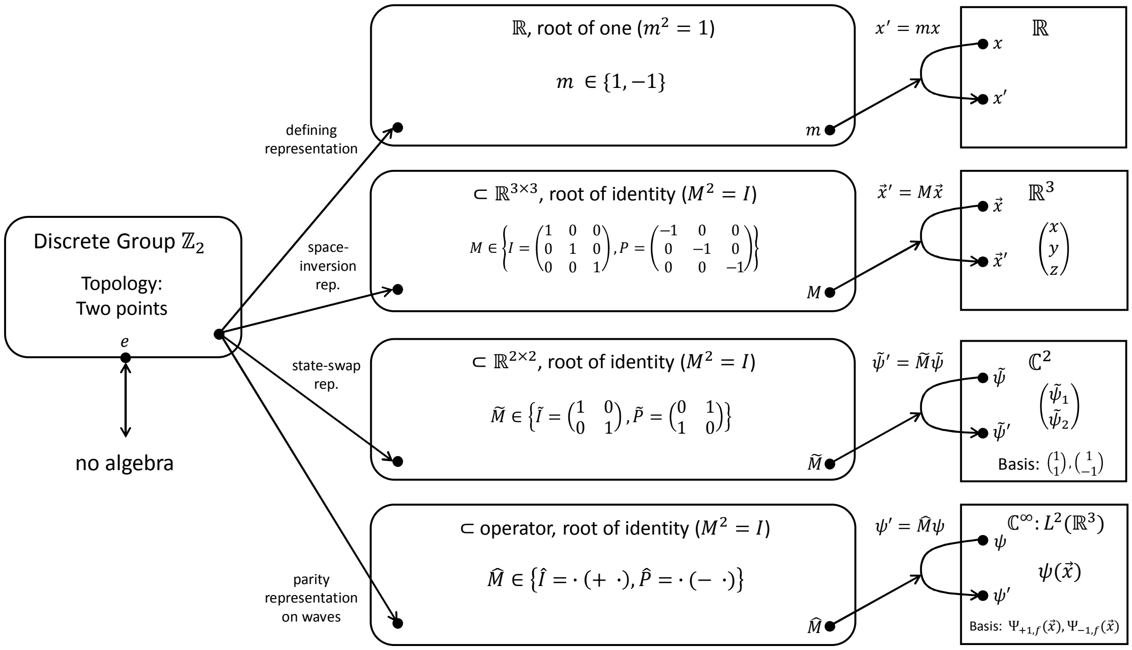
4.2 Z_2: The Cyclic Group of Order Two; Parity



The *cyclic group of order two*, $\mathbb{Z}_2$, contains only two elements, the identity and the reflection element: it is the simplest nontrivial group. We already met this group as a subgroup of the dihedral group D_3. We know that O(3) consists of the union of all proper rotations, that is, SO(3), and all improper rotations, that, is SO(3) followed by reflection. Now we can express this fact mathematically as O(3) = SO(3) × $\mathbb{Z}_2$. More generally, we can write O(n) = SO(n) × $\mathbb{Z}_2$ for odd n and O(n) = SO(n) ⋊ $\mathbb{Z}_2$ for even n (see https://en.wikipedia.org/wiki/Orthogonal_group). (Fun facts: SO(1) = {Identity} and O(1) = $\mathbb{Z}_2$, because the only possible length-preserving transformation in one dimension is a flip about the origin!)

The diagram shows four representations of this group. At the top is the defining 1-dimensional representation, which acts on real numbers. The two elements, identity and reflection, are mapped to the two integers, 1 and −1, respectively. An element, $m \in \{1, -1\}$, acts on the representation space by multiplication, $x' = mx$. Applying either element twice results in the identity: $m^2 = 1$. Thus m is a "root of one". Besides the trivial representation, this is the only irreducible representation of $\mathbb{Z}_2$.

The second representation from the top acts on 3-dimensional real vectors. It is the direct sum of three copies of the defining representations. The element $P = -I$, where I is the 3×3 identity matrix, reflects points of space (vectors) at the origin, $(x, y, z) \to (-x, -y, -z)$, an operation known as *space inversion* or *parity transformation*. Composing the proper rotations in O(3) with P yields the improper (reflected) ones. The related transformation $(x, y, z) \to (x, y, -z)$ is known as a *mirror reflection* (or *space reflection*) at the xy plane. It can be composed from a space inversion P and a 180° rotation about the z axis. (Similarly, there are mirror reflections at the yz and zx planes, which can be composed from P and rotations about the x and y axes, respectively.) But note that the transformation $(x, y, z) \to (-x, -y, z)$ is *not* a reflection, it is just a rotation by 180° about the z axis, an ordinary element of SO(3)!

The third representation from the top acts on a 2-dimensional (complex) quantum state, $\tilde{\psi} = (\tilde{\psi}_1, \tilde{\psi}_2)^T$. The element $\tilde{P}$ swaps the two components: $(\tilde{\psi}_1, \tilde{\psi}_2) \to (\tilde{\psi}_2, \tilde{\psi}_1)$. A good example for such a state is provided by the H_2^+ molecule, where the first basis state describes the electron near the first proton and the second basis state near the second proton [FLP, Vol. III, Ch. 17]. In this case, the state-swap operation is equivalent to a space inversion at the midpoint between the two protons.

The representation at the bottom acts on the single-particle wave function $\psi(\vec{x})$, a complex function of position in 3-dimensional space. The element $\hat{P}$ acts by reversing the sign of the argument $\psi(\vec{x}) \to \psi(-\vec{x})$. This is an infinite-dimensional representation constructed by applying the 3-dimensional space-inversion (or parity) representation to the wave function's argument.

We know that quantum observables correspond to generators of transformations. So, what are the generators of $\mathbb{Z}_2$? There is only one generator, namely the reflection element P: it can generate the only other element, $I = P^2$. If the reflection element represents a space inversion, as in our last three examples, the associated quantum observable P (no multiplication with $i\hbar$) is known as *parity*. Unlike angular momentum, parity has no classical analog: it is a purely quantum-mechanical observable. (The reflection element of $\mathbb{Z}_2$ could also represent time reversal, charge conjugation, exchange of identical particles, etc., but we won't discuss these possibilities and the related observables here.)

Let's work out the states of definite parity and their parity values for the two-state system in the third branch of the diagram. The matrix $\tilde{P}$ has two eigenvectors, $\tilde{\Psi}_{+1} = 1/\sqrt{2} \cdot (1,1)^T$ and $\tilde{\Psi}_{-1} = 1/\sqrt{2} \cdot (1,-1)^T$, with eigenvalues +1 and −1, respectively. The first eigenstate is known as the *even state* and the second one as the *odd state*. What does this mean for the electron in our H_2^+ molecule? In both eigenstates the electron is equally likely to be near proton 1 or proton 2, but the even state has parity +1 while the odd state has parity −1. The states of definite parity form a basis for the representation space, that is, we can write any state as $\tilde{\psi} = \alpha\tilde{\Psi}_{+1} + \beta\tilde{\Psi}_{-1}$ (see the diagram).

Next, let's look at the single-particle wave function in the bottom branch of the diagram. The operator $\hat{P}$ has infinitely many eigenfunctions, which can be divided into two groups: even functions for which $\psi(-\vec{x}) = \psi(\vec{x})$ and odd functions for which $\psi(-\vec{x}) = -\psi(\vec{x})$. All even functions have parity +1 and all odd functions have parity −1. For example, the *s*- and the *d*-waves in a hydrogen atom have parity +1, while the *p*-waves have parity −1 (assuming a single-electron wave function). Again, the wave functions of definite parity form a basis for the representation space: $\Psi_{+1,f}(\vec{x})$ with parity +1 and $\Psi_{-1,f}(\vec{x})$ with parity −1, where f labels basis functions within each group of functions (not specified here). Note that an arbitrary wave function $\psi(\vec{x})$ can always be decomposed into an even and an odd component $\psi(\vec{x}) = \psi_{+1}(\vec{x}) + \psi_{-1}(\vec{x})$, where $\psi_{+1}(\vec{x}) = \frac{1}{2}[\psi(\vec{x}) + \psi(-\vec{x})]$ and $\psi_{-1}(\vec{x}) = \frac{1}{2}[\psi(\vec{x}) - \psi(-\vec{x})]$.

If space inversion is a symmetry, then parity is a conserved quantity (i.e., P commutes with the Hamiltonian H). Moreover, if space inversion is a symmetry, then the states of definite parity are also states of definite energy (because P and H commute they have the same eigenvectors or eigenfunctions). (See the Appendix "Symmetry and Conservation in Quantum Mechanics".) For example, the H_2^+ molecule is symmetric under space inversion and therefore parity is conserved. Moreover, the even- and odd-parity states of the H_2^+ molecule correspond to definite-energy states with two different values [FLP, Vol. III, Ch. 10]. The hydrogen atom is also symmetric under space inversion and therefore parity is conserved as well. The even- and odd-parity states correspond to the definite-energy states of the *s*- *p*-, *d*- etc. orbitals.