

Before really working on Newns-Anderson model, the proper treatment of symmetries help us tremendously in the understanding of problems in physics and chemistry. For a many-particle system of identical particles, and this is what we usually deal with in the field of quantum gases, the symmetry under permutations of the particles is especially important.

0.1 Symmetrized states

For a system of N identical particles the Hamiltonian depends on the coordinates of all particles, however, owing to their indistinguishability the Hamiltonian can not change if we interchange the coordinates of two (or any number of) particles

$$H = H(1, 2, \dots, i, \dots, j, \dots, N-1, N) = H(1, 2, \dots, j, \dots, i, \dots, N-1, N), \quad (1)$$

where number $1, 2, \dots$ are shorthand for the coordinates (including spin, etc) of particle quantum numbers. (1) defines a *symmetry* of the Hamiltonian. More formally, the group of all permutations of N elements is called the symmetric group S_N . Now, we want to do something a bit abstract on system's wavefunction, i.e., we are looking for a transformation/representation.

Definition 0.1. A representation or a transformation \mathcal{R} is a map from a group G to the linear maps U in some vector space V

$$\begin{aligned} \mathcal{R} : G(V) &\rightarrow L(G(V)) \\ g &\rightarrow U(g), \end{aligned}$$

such that $U(g \circ h) = U(g) \circ U(h)$ where $g, h \in G$.

We could simply understand \mathcal{R} as a rotation operator(matrix) in vector space. It satisfies the linear mapping property even with associative property. However, our \mathcal{R} does not necessarily have later property. You will understand it from the following swapping operator which definitely violates associativity. Back to our many-body Hamiltonian, a natural way to such a representation is given by considering wave function $\psi(1, 2, \dots)$

$$P_{ij}\psi(1, 2, \dots, i, \dots, j, \dots, N-1, N) = \psi(1, 2, \dots, j, \dots, i, \dots, N-1, N) \quad (2)$$

Any permutation can be written as $P = \prod_{ij} P_{ij}$ and they all have the property $P_{ij}^2 = 1$. And hence the eigenvalues of P_{ij} are ± 1 as can be seen from

$$P_{ij}^2 \psi = P_{ij} \lambda \psi = \lambda^2 \psi \stackrel{!}{=} \psi \Rightarrow \lambda = \pm 1. \quad (3)$$

Let us recall the definition of an irreducible representation/transformation: It defines a subspace of the Hilbert space, which under the operation of any element g of the group G , transforms onto itself. Through the property $P_{ij}^2 = 1$ and the expression (2), it is evident that the symmetric group possesses irreducible representations of any dimension d . Let's delve into the derivation of this result.

In our case (2), we have two kinds of one dimensional representations take a special role: the symmetric and anti-symmetric wave functions

$$\begin{aligned} P_{ij}\psi_{s/a}(1, 2, \dots, i, \dots, j, \dots, N-1, N) &= \psi_{s/a}(1, 2, \dots, j, \dots, i, \dots, N-1, N) \\ &= \pm \psi_{s/a}(1, 2, \dots, i, \dots, j, \dots, N-1, N). \end{aligned} \quad (4)$$

By Schrodinger Equation, changing the sign of the wave function will not affect the Hamiltonian. And remind you that the group G in this case is Hamiltonian of the system instead of wave function. Therefore, (4) indicates that P_{ij} is a one-dimensional irreducible representation of S_N .

We call particles that are symmetric under permutations *bosons* and those that are anti-symmetric *fermions*.

0.2 Occupation Number Operator

In this section, we'll discuss occupation number states, which form the basis of the Newns-Anderson model. To delve deeper into this concept, we need to introduce the complementary approach for describing the many-particle system, focusing on the states of individual particles. And this states is normally noted as *single particle states*.

Definition 0.2. A single particle state of a many-particle system is given by

$$|i_1, \dots, i_N\rangle = |i_1\rangle_1 \otimes \dots \otimes |i_N\rangle_N, \quad (5)$$

where $|\cdot\rangle_j$ denotes the j th particle and i_j are the quantum number of the j th particle.

”single” in this context comes from that fact that we treat same type of particles in the system individually from (5). And *occupation number states* is one way doing it. It eliminates some of the dimensionality of the system by grouping particles with same quantum number. It is given by

$$|i_1, \dots, i_N\rangle = |n_1, n_2, \dots\rangle \quad (6)$$

Here n_i keep track of how many particles are residing in states i . And the total number of particles is given by

$$N = \sum_i n_i. \quad (7)$$

There are two important properties of these occupation states that follow directly from the single-particle states

$$1.) \langle n_1, n_2, \dots | n'_1, n'_2, \dots \rangle = \delta_{n_1, n'_1} \delta_{n_2, n'_2} \dots \quad (8)$$

$$2.) \sum_{n_1, n_2, \dots} |n_1, n_2, \dots\rangle \langle n_1, n_2, \dots| = 1 \quad (9)$$

The space of all occupation number states for all particle numbers N is called *Fock space*. Having this basis of properly symmetrized states at hand we would like to express all operators in it. A convenient way of doing so is by introducing creation and annihilation operators

$$\hat{a}_i^\dagger |\dots, n_i, \dots\rangle = \sqrt{n_i + 1} |\dots, n_i + 1, \dots\rangle, \quad (10)$$

$$\hat{a}_i |\dots, n_i + 1, \dots\rangle = \sqrt{n_i + 1} |\dots, n_i, \dots\rangle. \quad (11)$$

Back to the Bosons and Fermions context, we should have

$$[\hat{a}_i, \hat{a}_j] = \hat{a}_i \hat{a}_j - \hat{a}_j \hat{a}_i = [\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0, \quad [\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij} \quad \text{for bosons.} \quad (12)$$

It simply because of exchanging two bosons' state with each other will not affect the whole state from (4). In another word, $\hat{a}_i \hat{a}_j = \hat{a}_j \hat{a}_i$. Similarly for fermions, we have a slightly different result.

$$\{\hat{a}_i, \hat{a}_j\} = \hat{a}_i \hat{a}_j + \hat{a}_j \hat{a}_i = \{\hat{a}_i^\dagger, \hat{a}_j^\dagger\} = 0, \quad \{\hat{a}_i, \hat{a}_j^\dagger\} = \delta_{ij} \quad \text{for fermions.} \quad (13)$$

It dues to the fact that swapping two particles' state will result a extra $-$ on the whole state which leads to $\hat{a}_i \hat{a}_j + \hat{a}_j \hat{a}_i = 0$. A direct consequence of $\{\hat{a}_i^\dagger, \hat{a}_i^\dagger\} = 2\hat{a}_i^\dagger \hat{a}_i^\dagger = 0$ is the Pauli principle that states that no single particle state can be occupied by more than one fermion.