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Notes On Isotropy Subgroup Learning

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- In the lecture by H. Stokes, et al. introducing the isotropy subgroup (Click Me!), an important notion is the subspace of the distortion space. Given a specific distortion vector and operating all the group elements on the specified vector, all the distortion vectors we obtained automatically form a subspace – thus closed and self-consistent. The proof can be found in the following link: Click Me!

- The representation divide the whole distortion space to subspaces, and the isotropy subgroup divide the representation space (the aforementioned subspace) into sub-subspaces.

- Mathematically, the distortion space is composed by a whole bunch of distortion vectors. Basically, a specific distortion vector contains $3N$ coordinates, where N is the total number of atoms in the system. The aforementioned representation space (the subspace) refers to the group of distortion vectors that form a closed and self-consistent set. Since the representation space itself is a space, we can have the corresponding basis vectors and represent all the vectors in the subspace as a linear combination of the basis vectors. Then each vector in the subspace can be represented by a whole bunch of linear combination coefficients, and the number of the coefficients is just the number of basis vectors which is also the dimension of the subspace. Concerning the whole subspace is now represented by a whole bunch of linear combination coefficients, we now say the subspace is a *representation space*. For example, a 3D representation space can be written as a representation vector (a,b,c) which spans the whole 3D representation space. Then vectors like $(a,0,0)$ or $(a,b,0)$ is the 1D or 2D sub-subspace of the 3D representation space mentioned above.

- Here following is the link to a document introducing how to find the irreducible representations of a specific space group, based on the Bloch theorem – Click Me! Once the IR is pinned down, one can accordingly find the basis vectors spanning the representation space. The idea of looking of the basis vectors may be mathematically described as following:

  $$g\sum \eta_i \vec{a}_i = \sum \eta'_i \vec{a}_i \tag{0.1}$$

  where the representation space vector η transforms as following:

  $$\vec{\eta}' = D\eta \tag{0.2}$$

Here $\vec{\eta} = (\eta_1, \eta_2, \ldots)$, $\vec{\eta}' = (\eta'_1, \eta'_2, \ldots)$ and D is the representation matrix. Given the unknown basis vectors $\vec{a}_i$s, the equations 0.1 and 0.2 should be satisfied simultaneously. Therefore we can solve the equations to get the basis vectors. In some situations, we may not find the solution for $\vec{a}_i$s. This means we may not have the associated subspaces for a specific IR. For example, for the identity representation, we have all group elements represented by 1. Then we know that if there exists subspace associated with it, the subspace will definitely be one-dimensional. This means the subspace only contains one distortion vector, which further means that every group element operating on the only distortion vector in the subspace will bring it to itself (i.e. invariant). If it happens to be the case we don't have such a distortion vector, definitely the identity IR is not associated with any subspaces.

- Group element acting on the distortion vector is equivalent to representation matrix acting on the linear combination vector (the order parameter). Therefore in practice one tends to talk about the subject in the representation space. Once the IR is given, the representation space corresponding to certain subspace can be determined (if any). Then the division of the subspace into sub-subspaces can be specified with certain order parameter (e.g. the $(a, 0, 0)$ or $(a, b, 0)$, etc mentioned above). According to $D\eta = \eta$, all Ds satisfying such an equation forms a isotropy subgroup. In this sense, the establishing of the isotropy subgroup can be purely realized in the representation space without even specifying which subspace we are talking about (assuming we have multiple equivalent subspaces that are associated with the same IR).