Notes on Grain Boundary Basis Functions

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ABSTRACT

1 Introduction

The conventions and notes for generating basis function for the five-parameter grain boundary space are listed.

- Should we update `symm_orders` based on grain exchange symmetry and Laue group symmetry?.

    1. Before

- In the function, `null_mat_ab`, **In line 25, why am I dividing** `C_val` by `sqrt(2*e+1)` and **In line 29, how did I define the normalizing constant**. **Check with Jeremy!!**

1.1 Computing the Null Boundary Singularity Matrix

1.1.1 Description of `null_mat_ab.m`

The matrix `mat_ab` represents the null-boundary operation for fixed values of (a,b). The operation for null-boundary singularity is:

$$\sum_{ab}\sum_{\alpha\beta\gamma}\left[\Pi_{ab}C^{e-\varepsilon}_{a\alpha b\beta}C^{e0}_{a\gamma b-\gamma}\right]c^{ab}_{\alpha\beta\gamma}=\sqrt{2\pi^3}f_0\delta_{e0}\delta_{\varepsilon 0}$$

For fixed values of (a,b), the number of coefficients $c^{ab}_{\alpha\beta\gamma}$ is equal to $n_{col}=(2a+1)(2b+1)(2c+1)$, where $c=\min(a,b)$. Therefore, the number of columns of `mat_ab` is equal to n_{col}. The number of rows of of `mat_ab` is computed as follows:

- The values of e are constrained to lie between $|a-b|$ and $(a+b)$, i.e. $|a-b|\leq e\leq(a+b)$. These indices are stored in the variable `e_range`.
- For a given value of e, ε ranges from $-e$ to e. That is, $-e\leq\varepsilon\leq e$. This is provided by the variable `eps_range`.
- Therefore, the total number of rows is given by

$$n_{rows}=\sum_{e=|a-b|}^{a+b}\sum_{-e}^{e}\varepsilon$$

  This is given by the value in the expression `sum(2*e_range+1)` in line number 9.

- The Clebsch-Gordan coefficient is given by the function `clebsch_gordan(j1, j2, j, m)` for possible values of $C^{j,m}_{j1,m1;j2,m2}$. The function returns the coefficients `C` and the values of `m1` and `m2` for which $C^{j,m}_{j1,m1;j2,m2}\neq 0$.
- This function, `clebsch_gordan(j1, j2, j, m)`, is used to determine the indices containing non-zero values for a given row, `r_ct`. This is accomplished using the lines **20** and **23**.
  - In line **20**, the indices containing non-zero values for any fixed value of γ are computed.
  - In line **23**, the non-zero values are repeated for every value of γ. The corresponding indices are computed.
- **In line 25, why am I dividing** `C_val` by `sqrt(2*e+1)` and **In line 29, how did I define the normalizing constant**. **Check with Jeremy!!**

1.1.2 Description of `generate_gb_null.m`

This code computes the Null Boundary Operation for a range of (a,b) values provided in the `symm_orders` array. The matrix `null_mat` gives the operation for null-boundary singularity. The function `null_mat_ab` gives the operation for a fixed (a,b). However, we are interested in the operation for all possible values of (a,b) such that $\max(a+b) \leq N$ (N is denoted by the variable `Nmax`).

- The array `symm_orders` contains all the possible values of (a,b) such that symmetrized basis function (symmetrized using crystal rotation point group symmetries) exist.
- The variable `nsymm` gives the total number of basis functions $M^{a,b}_{\alpha,\beta,\gamma}$ for (a,b) values listed in `symm_orders`.
- The for-loop in lines **17** to **25** gives the appropriate row-indices (`row_inds`) and appropriate col-indices (`col_inds`), where the matrix operation computed using `null_mat_ab` will be added to the complete `null_mat`.
- Using the row- and column-indices computed in the previous for-loop, the for loop in lines **29** to **36**, calculates the `null_mat_ab` for each combination of (a,b) listed in `symm_orders` and add this to the matrix `null_mat`.

$$ {}_{\gamma}M^{a\ b}_{\alpha\ \beta} \tag{1} $$

References