Strategy to assign theoretical to the experimental muon site frequency

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Step 1: Set of distinct wyckoff positions P_β

Given a set of distinct wyckoff positions $P_T = \{P^1, P^2, \cdots P^M\} = \{P^\beta\}_{\beta=1}^{M}$, where M is the number of inequivalent positions. Each element P_β of the set is associated distinct wyckoff positions and its total Energy E_β. For simplicity we chose $E_1(P^1) < E_2(P^2) < \cdots < E_M(P^M)$. Thus, P^β's are arranged in ascending order of energies.

Step 2: Symmetry search

Suppose, for each position $P_\beta \in P_T \; \exists \; P_\beta = \{p_\alpha^\beta\}_{\alpha=1}^{N_\beta}$, where $N_\beta \geq 1$(and $\beta = 1, 2, 3, \cdots M$) is the number of magnetically inequivalent positions p_α^β (wyckoff sites). In a magnetic systems, magnetic order generates a local magnetic field at the muon position which breaks the crystal symmetry that generates $\{p_\alpha\}$, i.e. the wyckoff sites separates into N_α magnetically inequivalent sites. Thus, P_T

$$\{p_\alpha^\beta\} = \begin{Bmatrix} p_1^1 & p_2^1 & \cdots & p_{N_\beta}^1 \\ p_1^2 & p_2^2 & \cdots & p_{N_\beta}^2 \\ \vdots & \vdots & \ddots & \vdots \\ p_1^M & p_2^M & \cdots & p_{N_\beta}^M \end{Bmatrix} = \begin{Bmatrix} P^1 \\ P^2 \\ \vdots \\ P^M \end{Bmatrix} \tag{1}$$

where Eqn. (1) is not a square or a rectangular matrix but rather we call it a "*Ladder matrix*" of set positions for the time being.

Step 3: Dipolar fields d_i

Now, for each position P_β we can compute a set of dipolar frequencies, $D_i = \{d_j^i\}$ ($i = 1, 2, \cdots M, j = N_1, N_2, \cdots N_M$), where $N_1, N_2, \cdots N_M$) is the number of magnetically

inequivalent sites for each $P_1, P_2, \cdots P_M$, respectively. This can be easily visualized as a Ladder matrix of dipolar fields

$$\begin{Bmatrix} d_1^1 & d_2^1 & \cdots & d_{N_1}^1 \\ d_1^2 & d_2^2 & \cdots & d_{N_2}^2 \\ \vdots & \vdots & \ddots & \vdots \\ d_1^M & d_2^M & \cdots & d_{N_M}^M \end{Bmatrix} = \begin{Bmatrix} D^1 \\ D^2 \\ \vdots \\ D^M \end{Bmatrix} = D \tag{2}$$

Step 4: collaps d_i

Given the list of real frequencies say $D^i = \{d_1^i, d_2^i, \cdots d_{N_i}^i\}$, we can compute

$$\Delta D_i[j] = D_i^{\text{sort}}[j+1] - D_i^{\text{sort}}[j] \tag{3}$$

$$\overline{D_i}[j] = \frac{D_i^{\text{sort}}[j+1] + D_i^{\text{sort}}[j]}{2} \tag{4}$$

$$\delta D_i[j] = \frac{\Delta D_i[j]}{\overline{D_i}[j]} \quad (i = 1, 2 \cdots M, j = 1, 2 \cdots N_i) \tag{5}$$

where D_i^{sort} is the sorted list of D_i. We collapse the m consecutive values D_i whose ratio $\delta D_i[j]$ are smaller than the threshold δ. This produces $n_i \leq N_i$ distinct new values that we label as $\overline{D_i}$. This procedure will be done for D_i's to generate a new Ladder matrix of average dipolar fields with elements define as

$$\overline{d}_k^i = \sum_{j=k}^{k+m} \frac{d_j^i}{m} \quad ; (j = 1, 2 \cdots N_i, k = 1, 2, \cdots n_i) \tag{6}$$

$$\begin{Bmatrix} \overline{d_1}^1 & \overline{d_2}^1 & \cdots & \overline{d}_{n_1}^1 \\ \overline{d_1}^2 & \overline{d_2}^2 & \cdots & \overline{d}_{n_2}^2 \\ \vdots & \vdots & \ddots & \vdots \\ \overline{d_1}^M & \overline{d_2}^M & \cdots & \overline{d}_{n_M}^M \end{Bmatrix} = \begin{Bmatrix} \overline{D_1} \\ \overline{D_2} \\ \vdots \\ \overline{D_M} \end{Bmatrix} = \overline{D} \tag{7}$$

Note: the matrix Eqn. (7) also only contains the values that certify the condition of $\delta D_i > \delta$.

Step 4: Sorting $\overline{d_k}^i$

Next, we sort out all the element of $\{\overline{d_k}^i\}$ in ascending values and create a sequence Φ where values of different wyckoff sites β (having n_β magnetically inequivalent positions) are inter-dispersed as

$$
\begin{aligned}
\Phi &= \{\overline{d_\gamma}\}_{\gamma=1}^{L} = \{\overline{d_\alpha}^{\beta}\}_{\text{sorted}}, \\
\alpha &\in \{1, 2, \cdots n_\beta\}, \\
\beta &= 1, 2, \cdots M, \\
\gamma &= 1, 2, \cdots L \\
\text{where } L &= \sum_{\beta}^{M} n_\beta
\end{aligned}
\tag{8}
$$

Step 5: Theoretical pairing with Experimental data

Given a list of value of experimental data arranged in ascending order: say $\Omega = \{\omega_1, \omega_2, \cdots \omega_M\} = \{\omega_k\}_{k=1}^{M}$ for a given material, where M is the number of experimental frequencies. Thus, we can assign each of theoretical values of Φ to the experimental data $\Omega = \{\overline{d_\gamma}\}_{\gamma=1}^{L}$ as.

a) **pairing** as

$$
\begin{aligned}
\omega_1 &\longrightarrow \overline{d_1} \\
\omega_2 &\longrightarrow \overline{d_2} \\
&\cdots \\
\omega_Z &\longrightarrow \overline{d_\ell} \\
\text{where } \ell &= \min\{L, M\}
\end{aligned}
\tag{9}
$$

NOTE: ℓ details whether or not all the experimental data are pair with the calculated value (see figure 1), and

b) **the best match** which we can be represented in terms of graph theory (see figure 1). Lets look at the experimental (Ω) and and calculated (Φ) values as if they were a bipartite graph, where each edge between the ith experimental value and jth calculated value has weight define for each ith as $C_{ij} = |\omega_i - \overline{d_j}|$. Then our task is to find minimum-weight matching in the graph that will assigned each ω_i's to $\overline{d_j}$'s. This problem is known become an assignment problem which can be solve by Hungarian method (or Kuhn-Munkres method). The Biparted graph as shown in figure 1 can be converted to Adjacency matrix for the assignment problem which can be solve with linear assignment problem implemented on `SciPy:scipy.optimize.linear_sum_assignment(cost_matrix, maximize=False)`, where `cost_matrix` is the matrix we refer to as C_{ij} which can extracted for example from figure 1 as

$$
C_{ij} = \begin{pmatrix}
|\omega_1 - \overline{d_1}| & |\omega_1 - \overline{d_2}| & |\omega_1 - \overline{d_3}| & |\omega_1 - \overline{d_4}| \\
|\omega_2 - \overline{d_1}| & |\omega_2 - \overline{d_2}| & |\omega_2 - \overline{d_3}| & |\omega_2 - \overline{d_4}| \\
|\omega_3 - \overline{d_1}| & |\omega_3 - \overline{d_2}| & |\omega_3 - \overline{d_3}| & |\omega_3 - \overline{d_4}|
\end{pmatrix}
\tag{10}
$$

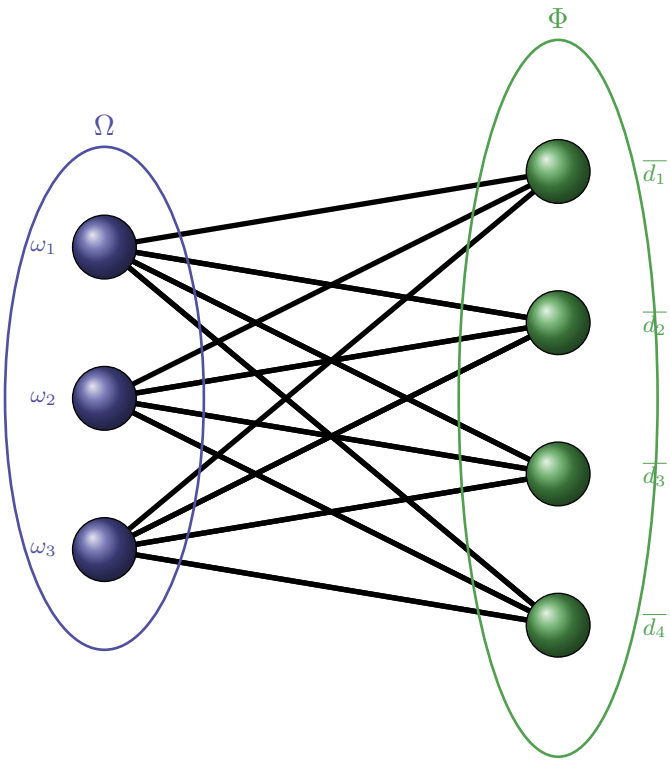

Figure 1: Biparted graph to show relation ship between the experimental values $\Omega = \{\omega_i\}_{i=1}^{M}$ and calculated values $\Phi = \{\overline{d_j}\}_{j=1}^{L}$, where edges are the weight defined as $C_{ij} = |\omega_i - \overline{d_j}|$.

Bipartite graphs and the Hungarian algorithm

Bipartite graphs

- when two set of vertices say Ω and Φ are completely separated from one another
- can be **connected** i.e. every vertex in Ω would connect to every vertex in Φ (see figure 1), but this doesn't always have to be the case
- all tree diagram can be considered bipartite
- bipartite graphs can be weighted (as in equation 10) i.e a value that represent the connection between the vertex and can be anything like a cost, time etc. to perform a particular task.
- can be used to solve an "allocation problems" as an effective way to utilise network between Ω and Φ
- to solve allocated problems we convert our weighted bipartite graph in to a matrix in equation 10, and the best way to do that is using Hungarian algorithm

Hungarian algorithm

References