FRITZ-HABER-INSTITUT
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Symmetry in Physical Problems: A Linear Algebra Approach

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Overview

Goals

- **Symmetry** in solid state physics **is basic linear algebra**
- impose relevant symmetries on physical models
- use symmetries to reduce dimensions of tensors

This talk

- introduce mathematical background and necessary tools
- present the **key ideas** without being too technical
- ➔ **Example script illustrating everything is available**

Discussion?

Symmetry – Examples

Global symmetries

- Permutation symmetry (Transposition)

$$H = H^{\mathrm{T}}$$

- Absolute location in space (rigid translations)

$$E(x + \mathrm{d}x) = E(x)$$

- Absolute orientation in space (rigid rotations)

$$H = M\,H\,M^{\mathrm{T}}$$

Point group symmetry in molecules

- **Finite** rotations and reflections in molecules

Space group symmetry in crystals

- **Finite** rotations, reflections **and translations**

Vectorization – Definition

Problem: Find common language to express symmetries

$$H = H^{\mathrm{T}}$$
$$H = M\,H\,M^{\mathrm{T}}$$

Solution: **Vectorize** expressions

Vectorization

$$\begin{aligned} \mathbf{vec} \;:\; \mathbb{R}^{D\times D} &\longrightarrow \mathbb{R}^{D^2\times 1} \\ \mathbf{vec}\,H &\longmapsto \boldsymbol{h} \end{aligned}$$

$$\begin{aligned} \mathrm{unvec} \;:\; \mathbb{R}^{D^2\times 1} &\longrightarrow \mathbb{R}^{D\times D} \\ \mathrm{unvec}\,\boldsymbol{h} &\longmapsto H \end{aligned}$$

Vectorization – Why it is useful

Transposition

$$H = \begin{bmatrix} a & c \\ b & d \end{bmatrix} ,$$

$$\boldsymbol{h} = \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} ,$$

$$T\boldsymbol{h} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \begin{pmatrix} a \\ c \\ b \\ d \end{pmatrix} ,$$

$$\rightarrow \text{unvec}\,(T\boldsymbol{h}) = \begin{bmatrix} a & b \\ c & d \end{bmatrix} = H^T .$$

Vectorization – Why it is useful

Roth's Relationship

$$\mathbf{vec}\,(ABC) = (C^{\mathrm{T}} \otimes A)\,\mathbf{vec}\,B$$
$$\Longrightarrow \quad \mathbf{vec}\,(M\,H\,M^{\mathrm{T}}) = (M \otimes M)\,\mathbf{vec}\,H$$

Conclusion:
Relations relevant to express symmetries of a given tensor H, e. g., transposition and rotation, can be stated as plain **matrix multiplications** in the **vectorized representation** of the tensor H:

$$\boldsymbol{h} = T_{[D^2 \times D^2]}\,\boldsymbol{h}$$
$$\boldsymbol{h} = (M \otimes M)_{[D^2 \times D^2]}\,\boldsymbol{h}$$
$$\vdots$$

Construction of the Invariant Space

Sum up the constraints of interest

$$
\begin{aligned}
\boldsymbol{h} &= M_1\,\boldsymbol{h} \\
\boldsymbol{h} &= M_2\,\boldsymbol{h} \\
&\vdots \\
\Leftrightarrow \sum_i (\mathbb{1} - M_i)\,\boldsymbol{h} &= 0
\end{aligned}
$$

Conclusions:

- $\boldsymbol{h}$ lies in the **kernel** or **nullspace** of

$$
\mathbb{M} = \sum_i (\mathbb{1} - M_i)
$$

→ Obtain $\ker(\mathbb{M})$ by performing **SVD** on $\mathbb{M}$ (see example script)

→ The **dimension** of $\ker(\mathbb{M})$ gives the **number of irreducible components** $\tilde{\boldsymbol{h}}$ of $\boldsymbol{h}$ and thus h.

Construction of the Invariant Space

Build projectors from span of $\ker(\mathbb{M})$

- S contains the basis vectors of $\ker(\mathbb{M})$

$$\boldsymbol{h} = S\tilde{\boldsymbol{h}}$$

- S^{T} maps to irreducible components

$$\tilde{\boldsymbol{h}} = S^{\mathrm{T}}\boldsymbol{h}$$

- SS^{T} is projector that can be used to symmetrize

Example: Symmetrize matrix (see example script)

$$\begin{bmatrix} a & c \\ b & d \end{bmatrix} \overset{\textbf{vec}}{\Longrightarrow} \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} \overset{S^{\mathrm{T}}}{\Longrightarrow} \tilde{\boldsymbol{h}} = \begin{pmatrix} \tilde{a} \\ \tilde{b} \\ \tilde{c} \end{pmatrix} \overset{\mathrm{unvec}\,(S\tilde{\boldsymbol{h}})}{\Longrightarrow} \begin{bmatrix} a & \frac{1}{2}(b+c) \\ \frac{1}{2}(b+c) & d \end{bmatrix}$$

Application: Vibrational Modes

From finite differences or Molecular Dynamics

- Set of displacements

$$U = (\boldsymbol{u}_1, \ldots, \boldsymbol{u}_N)$$

- Set of forces

$$F = (\boldsymbol{f}_1, \ldots, \boldsymbol{f}_N)$$

→ Find

$$F = HU\,,$$

with H the *effective* **Hessian** of the system.

Solve with **Moore-Penrose Inverse** U^+

$$H = FU^+$$

Equivalent to **least squares solution** for $\mathbf{vec}\,H$ in

$$\mathbf{vec}\,F = (U^\mathrm{T} \otimes \mathbb{1})\,\mathbf{vec}\,H$$

Vibrational Modes in CO_2 and H_2O

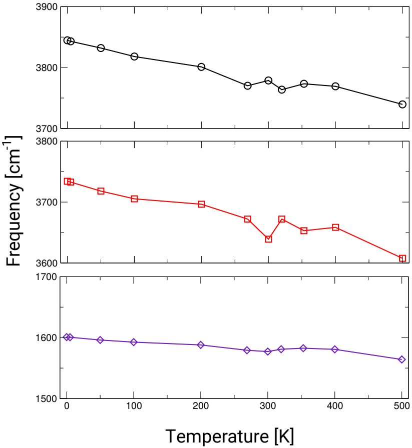
H_2O: PBE, NVT, $\mathrm{d}t$=0.5 fs, τ=0.05 ps, T=2 ps, 500 fs discarded

Mode	Fin. diff.	(sym)	Fit at 5 K	(sym)
1	3845	3845	3843	3843
2	3734	3734	3732	3733
3	1601	1601	1601	1601
4	**3**	**0**	**1342**	0
5	**3**	**0**	0	0
6	**3**	**0**	0	0

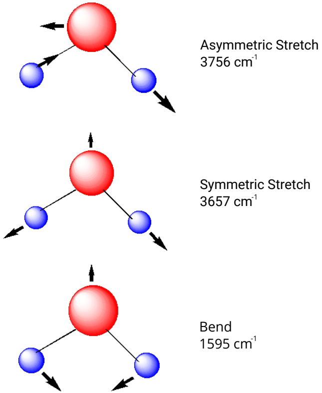
CO_2: PBE, NVT, $\mathrm{d}t$=1 fs, τ=0.05 ps, T=2 ps, 500 fs discarded

Mode	Fin. diff	(sym)	Fit at 5 K	(sym)
1	2368	2368	2367	2367
2	1322	1322	**1520**	1322
3	**633**	**633**	1322	634
4	**634**	**0**	634	0
5	0	0	0	0

Temperature Dependence of Modes



Change of vibrational frequencies with temperature



Sketch of Vibrational modes
`physics.stackexchange.com/a/153091`

Outlook

Can we do more than molecules with few atoms? **Yes!**

- Higher order force constants
- Supercells with $\mathcal{O}(100)$ atoms
- Reduce dimensionality:
  - bcc, 4x4x4 supercell (128 atoms): **147 456** components in H
  - ➔ Exploit symmetry: **11** irreducible components

What else?

- Symmetry constrained relaxation
- Freeze out modes during molecular dynamics?

Who came up with this?

- Olle Hellman (Caltech)
- ➔ Check out: `ollehellman.github.io`

Q & A

- Is the change of vibrational modes in water an artifact of the fit or a measurable effect (neglecting something like nuclear quantum effects etc.)?
- How do use symmetry?