Brian Busemeyer
General notes from research
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# Contents



# 1 Symmetry and the Hamiltonian

Symmetries are quite helpful in coarse graining, because they limit the number of possible model possible model parameters. Given an operator $O$ that commutes with a symmetry operator $S$, e.g. $[O, S] = 0$, there are a number of benefits that occur when choosing to express $O$ in terms of eigenstates of $S$. As shown below, many terms of $O$ in the basis of eigenstates of $S$ are zero. Additionally many of the terms of $O$ will be constrained to be equal. This usually means that $O$ is either sparse, or representable with only a few free parameters.

## 1.1 One-body terms that are zero by symmetry

For a one-body Hamiltonian, the space is all just one-body states. Let $\mathcal{H}$ be that Hamiltonian, and $S$ be a symmetry operator. If $\mathcal{H}$ is invariant to that symmetry,

$$[\mathcal{H}, S] = 0$$

You can show that this implies $\mathcal{H}$ is block-diagonal in the eigenstates of $S$. Let $\phi_i$ have the property that $S\phi_i = \lambda_i \phi_i$. Then $S(\mathcal{H}\phi_i) = \lambda_i(\mathcal{H}\phi_i)$, using the commutator. This implies that $\mathcal{H}\phi_i$ is a state in the degenerate subspace of $\phi_i$.

Let $S\phi_j = \lambda_j \phi_j$, and $\lambda_j \neq \lambda_i$. Then

$$\langle \phi_j | \mathcal{H}\phi_i \rangle = 0$$

if $\phi_j$ is orthogonal to all the eigenstates of a different eigenvalue. Is it possible to show that this is true for any possible $S$?

### 1.1.1 Example

Consider the model Hamiltonian,

$$\mathcal{H}_{\text{eff}} = \sum_i \epsilon_i n_i + \sum_{ij} t_{ij} c_i^\dagger c_j$$

The matrix representation of this model is $\epsilon_i \delta_{ij} + (1 - \delta_{ij}) t_{ij}$.

Consider if you have an orthonormal basis of eigenstates of a symmetry operator $S$, where $[\mathcal{H}, S] = 0$. Consider if this is the basis of $\mathcal{H}_{\text{eff}}$. This requires that $t_{ij} = 0$ between eigenstate of $S$ with different eigenvalues.

## 1.2 Symmetry-related terms

Consider if $[\mathcal{H}, S] = 0$ for some symmetry operator $S$.

$$[\mathcal{H}, S] = 0 \iff \mathcal{H}S - S\mathcal{H} = 0 \iff S^{-1}\mathcal{H}S = \mathcal{H}$$

If $S$ represents a change of basis, such as a unitary operator, then this suggests that $\mathcal{H}$ is invariant to the change of basis represented by $S$.

Now let $\phi_i$ be some basis for $\mathcal{H}$, Then

$$\langle \phi_i | \mathcal{H} | \phi_j \rangle = \langle S\phi_i | \mathcal{H} | S\phi_j \rangle$$

Thus, the element is the same as the element relating the basis set elements generated by $S$. In particular, if $S\phi_i = \phi_i$ and $S\phi_j = \phi_k$, then $\langle \phi_i | \mathcal{H} | \phi_j \rangle = \langle \phi_i | \mathcal{H} | \phi_k \rangle$.

### 1.2.1 Example of symmetry-related terms

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For the FeSe diatomic molecule, oriented along the $\hat{z}$, for $S$ as rotation about $\hat{z}$ by $\pi/8$, the Se $s$ state is invariant and the $d_{x^2-y^2}$ is mapped to $d_{xy}$. Thus the hopping element between the $s$ and $d_{x^2-y^2}$ is the same as the hopping to $d_{xy}$.

Another example: nearest neighbor hopping terms are all the same between the same atomic pairs by translational symmetry.