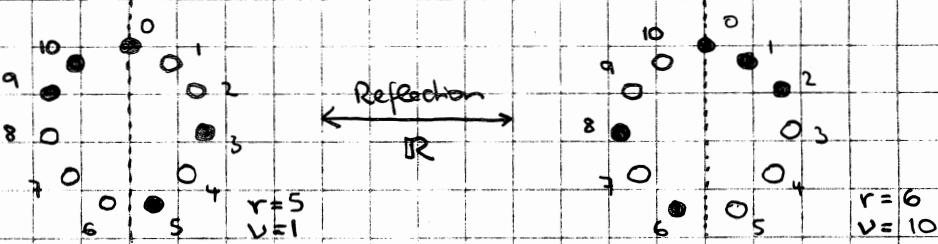


The Diffusion Problem: Symmetry Properties

(a) The reflection Operation

Two atomic arrangements that transform into each other when the contents of the sites k and $(p-k) \bmod p$ are exchanged ($k=0, 1, 2, \dots, p-1$) are by definition images of each other under the mirror reflection operation R :



Some basic properties of the reflection operation can be immediately established:

- (i) The site 0 is a fixed element under the reflection operation for odd numbers of sites p . (For prime p , $p \geq 3$.)
- (ii) The block number m is an invariant under R . [See the script on equilibrium properties.]
- (iii) The pattern sum r [see the script on diagonalization i page 4,6] changes under reflections as:

$$\begin{aligned}
 r[R(e)] &= [(p-v_1) + (p-v_2) + \dots + (p-v_k)] \bmod p \\
 &= [-v_1 - v_2 - \dots - v_k] \bmod p \\
 &= -r[e]
 \end{aligned} \tag{1}$$

where e is a configuration with k atoms located at the sites v_1, v_2, \dots, v_k .

As a consequence, primitives β (configurations with vanishing pattern sum $r=0$) are transformed into primitives $R[\beta]$.

(iv) Two-fold application of the reflection operation reproduces the original arrangement: $R^2 = \mathbb{1}$.

This implies that the eigenvalues λ of R must fulfil $\rho^2 = 1$, i.e., $\rho = \pm 1$ holds.

(b) Symmetric and antisymmetric eigenspaces

Under reflections, a clockwise jump transforms into a counter-clockwise jump, while the type of the jump event does not change. Since the rates of the individual jumps do not depend on their direction, an initial configuration and its mirror image will evolve identically, i.e., remain images of each other under reflection at all times.

Mathematically spoken, this means that the Liouville operator \mathcal{L} (right hand-side matrix) in eq. (17) [script on diagonalization] must commute with the reflection operator R :

$$\frac{d}{dt} \langle [\gamma_l | v] \rangle = \sum_{[z_l | \mu]} \mathcal{L}_{[\text{Eng}(v), [z_l | \mu]]} \langle [z_l | \mu] \rangle \quad (1)$$

$$\mathcal{L}R = R\mathcal{L} \quad (2)$$

This means that all non-degenerate eigenvectors \vec{u} of \mathcal{L} , $\mathcal{L}\vec{u} = \lambda\vec{u}$, must also be eigenvectors of R . To prove this assertion, we note that with (2),

$$R\mathcal{L}\vec{u} = R\lambda\vec{u} = \lambda R\vec{u} \quad (3)$$

so $R\vec{u}$ is an eigenvector of \mathcal{L} with the same eigenvalue λ , and thus a multiple of \vec{u} , if the eigenvector is non-degenerate:

$$R\vec{u} = \rho\vec{u} = \pm\vec{u} \quad (4)$$

These eigenvalues and eigenvectors thus may be labelled symmetric and antisymmetric, respectively.

(3)

The equilibrium eigenvector \vec{u}_{eq} with eigenvalue $\lambda=0$ presents a prominent example. Conservation of probability enforces the normalization (where $\vec{n} = (\dots 1 \ 1 \ 1 \dots)^T$ is a vector of unit entries):

$$\vec{n}^T \cdot \vec{u}_{\text{eq}} = 1 \quad (5)$$

since there is unit probability to find the system in an arbitrary configuration. Now, note that $R = R^+$ is a hermitian operator (because it only exchanges pairs of states), and $R \cdot \vec{n} = \vec{n}$ (entries for states and their mirror images are trivially identical here). Hence, we find:

$$\vec{n}^T \cdot \vec{u}_{\text{eq}} = (R \vec{n})^T \cdot \vec{u}_{\text{eq}} = \vec{n}^T (R \vec{u}_{\text{eq}}) = 1 \quad (6)$$

which implies $R \vec{u}_{\text{eq}} = \vec{u}_{\text{eq}}$. The equilibrium eigenvector is always symmetric, if it is non-degenerate.

In the case of degenerate eigenvalues of \mathcal{L} , the notion of projectors P_S, P_A onto the symmetric and antisymmetric subspaces of R is helpful. They are defined via:

$$P_S = \frac{1}{2} (I + R), \quad P_A = \frac{1}{2} (I - R) \quad (7)$$

and have the obvious properties:

$$P_S + P_A = I, \quad P_S - P_A = R$$

$$P_S^2 = P_S, \quad P_A^2 = P_A, \quad P_S P_A = P_A P_S = 0 \quad (8)$$

$$R P_S = P_S, \quad R P_A = -P_A$$

P_S and P_A thus effectively decompose any vector \vec{w} into a symmetric and an antisymmetric part \vec{w}_S, \vec{w}_A :

$$\begin{aligned} \vec{w}_S &= P_S \vec{w}, & R \vec{w}_S &= \vec{w}_S \\ \vec{w}_A &= P_A \vec{w}, & R \vec{w}_A &= -\vec{w}_A \\ \vec{w} &= \vec{w}_S + \vec{w}_A, & R \vec{w} &= \vec{w}_S - \vec{w}_A \end{aligned} \quad (9)$$

Because with (2) also P_S and P_A commute with \mathcal{L} , reasoning similar to (3) and (4) shows that with every eigenvector \vec{u} of \mathcal{L} , $\mathcal{L}\vec{u} = \lambda\vec{u}$, also its projections $\vec{u}_S = P_S\vec{u}$ and $\vec{u}_A = P_A\vec{u}$ are eigenvectors of \mathcal{L} :

$$\mathcal{L}\vec{u}_S = \mathcal{L}P_S\vec{u} = P_S\mathcal{L}\vec{u} = \lambda P_S\vec{u} = \lambda\vec{u}_S \quad (10)$$

and analogously for \vec{u}_A . According to (9), \vec{u}_S and \vec{u}_A are vectors of definite symmetry under reflections R . In particular, if λ is an eigenvalue of \mathcal{L} with twofold degeneracy, then either the whole eigenspace is symmetric or antisymmetric, or the symmetric and antisymmetric vectors $\vec{u}_S = P_S\vec{u}$ and $\vec{u}_A = P_A\vec{u}$ form a unique base set of definite symmetry — apart from their normalization, the vectors \vec{u}_S and \vec{u}_A are independent of the choice of "generating" eigenvector \vec{u} of \mathcal{L} .

(c) Dimension of the eigenspaces; palindromic states

Next, we inquire into the number of linearly independent states in both the symmetric and antisymmetric eigenspaces of R . In this context, it is useful to examine the primitive configurations separately.

(i) Non-primitive configurations. These include all arrangements that are rotationally equivalent to some primitive \vec{z} , but are rotated with respect to it by a shift $v \neq 0$ [see page 8, script on diagonalization]. Under the reflection operation R , one obtains a pattern that belongs to the equivalence class of the mirror image $R[\vec{z}]$ of the primitive ($R[\vec{z}]$ is itself primitive; see Section (a), (iii)), with a rotational shift $-v \bmod p$.

Now, for odd p (p prime, $p \geq 3$), $v \bmod p$ and $-v \bmod p$ are always different if $v \neq 0$, since:

$$v \bmod p - (-v \bmod p) = (2v) \bmod p \neq 0 \quad (11)$$

(Otherwise, p would be evenly divisible by 2!) Hence, the mirror image of $[\vec{z}|v]$, i.e. $[R[\vec{z}]| -v]$, is always different from the original if $v \neq 0$: Non-primitive configurations

always come in pairs of mirror images. These pairs are obviously mutually exclusive.

Denoting the unit probability vector that places the system in the configuration $[z|v]$ by $\vec{e}_{[z|v]}$, two eigenstates of IR with definite symmetry are generated by the projectors P_S and P_A :

$$\vec{e}_{[z|v]}^{(S)} = P_S \vec{e}_{[z|v]} = \frac{1}{2} (\vec{e}_{[z|v]} + \vec{e}_{[Rz|1-v]}) \quad (12)$$

$$\vec{e}_{[z|v]}^{(A)} = P_A \vec{e}_{[z|v]} = \frac{1}{2} (\vec{e}_{[z|v]} - \vec{e}_{[Rz|1-v]})$$

Note that $\vec{e}_{[z|v]}^{(S)} = \vec{e}_{[Rz|1-v]}$ and $\vec{e}_{[z|v]}^{(A)} = -\vec{e}_{[Rz|1-v]}$; the non-primitive configurations therefore give rise to:

$$\frac{1}{2}(p-1) N_{\text{prim}} = \frac{p-1}{2p} \binom{p}{k} \quad (13)$$

symmetric and antisymmetric base states each (see eq. (2), script on diagonalization).

(iii) Primitive configurations. If the initial configuration z is primitive, so will be its mirror image $R[z]$. This presents two different situations:

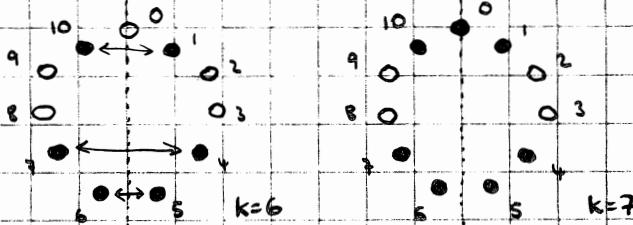
- (α) z and $R[z]$ are distinct primitives,
- (β) z and $R[z]$ are identical.

The case (α) is completely analogous to the situation encountered in section (i); the projectors P_S and P_A again deliver a pair of states $\vec{e}_{[z|0]}^{(S)}$, $\vec{e}_{[z|0]}^{(A)}$ of definite symmetry coupling the entries for $[z|0]$ and $[Rz|0]$ (12). The case (β) warrants special attention, however.

(iii) Palindromic states. A configuration z that is its own mirror image under reflections IR will be called palindromic. Obviously, all palindromic states are primitive, and the unit vectors $\vec{e}_{[z|0]}$ associated with them are symmetric under reflections: $\text{IR} \vec{e}_{[z|0]} = P_S \vec{e}_{[z|0]} = \vec{e}_{[z|0]}$, as (12) shows at once.

Palindromic configurations thus generate only symmetric states.

The number of palindromic primitives can be determined as follows: Consider a circular arrangement as shown in the figure:



In a palindromic arrangement, the occupation status of the pairs of sites $\nu, \rho-\nu$ must be the same, while the occupation of site 0 is not restricted any further. (Clearly, the pattern sum r of patterns constructed in this fashion always vanishes, rendering them primitive.) This means that we are free to distribute half of the atoms on the half-circle of sites $1, 2, \dots, \frac{p-1}{2}$; the location of the remaining half is fixed by the symmetry requirement. If the number of atoms k is odd, the single unpaired atom will populate the unrestricted site 0. The number of arrangements is thus given by :

$$N_{\text{palindrom}} = \binom{(p-1)/2}{k/2} \quad (k \text{ even}) \quad (14)$$

$$N_{\text{palindrom}} = \binom{(p-1)/2}{(k-1)/2} \quad (k \text{ odd})$$

The total number of symmetric and antisymmetric states then follows from (13), (14):

$$N_{\text{symm}} = \frac{1}{2} \binom{p}{k} + \frac{1}{2} N_{\text{palindrom}} \quad (15)$$

$$N_{\text{anti}} = \frac{1}{2} \binom{p}{k} - \frac{1}{2} N_{\text{palindrom}}$$

(d) Reflection symmetry and momentum space

We introduced momentum states ($z|q\rangle$) (17) in the script on diagonalization as a means to decouple the master equation describing the evolution of the system. Here, we explore how

$$\begin{aligned}\langle (\bar{z}|0)_S \rangle &= \frac{1}{P} \sum_{v=0}^{P-1} \tilde{e}_{[\bar{z}|v]}^{(S)} = \frac{1}{2P} \sum_{v=0}^{P-1} \langle [\bar{z}|v] + [R[\bar{z}]|v] \rangle \\ \langle (\bar{z}|0)_A \rangle &= \frac{1}{P} \sum_{v=0}^{P-1} \tilde{e}_{[\bar{z}|v]}^{(A)} = \frac{1}{2P} \sum_{v=0}^{P-1} \langle [\bar{z}|v] - [R[\bar{z}]|v] \rangle\end{aligned}\quad (20)$$

(see (12)), one may diagonalize the decay coefficient matrix $R(0)$ [eq. (25), script on diagonalization] separately in the symmetric and antisymmetric subspaces $\langle (\bar{z}|0)_S \rangle = \langle (P_S[\bar{z}]|0) \rangle$, $\langle (\bar{z}|0)_A \rangle = \langle (P_A[\bar{z}]|0) \rangle$. In other words, $R(0)$ is reducible and in the symmetric-antisymmetric base, is a block-diagonal matrix. This property could be exploited in numerical diagonalization schemes.

In this context, we also note that with $R(0)$, also the symmetrized matrix $\tilde{R}(0) = S^{-1}R(0)S$ [eq. (41), diagonalization script] commutes with the reflection operator R : $R\tilde{R}(0) = \tilde{R}(0)R$. This is because the reflection operator merely exchanges a primitive with its mirror image, both of which share the same occupation $\rho_{\text{eq}}(\bar{z}) = \rho_{\text{eq}}(R[\bar{z}])$ in equilibrium. Thus, the diagonal matrix S [eq. (40), diagonalization script], and R commute, $SR = RS$, from which eq. (4) follows immediately. As a consequence, we may select an orthonormal base of eigenvectors of $\tilde{R}(0)$ to compose the orthogonal transformation matrix $U(0)$ [eq. (41), diagonalization script] that contains

$$N_{\substack{\text{symm} \\ \text{anti}}}^{(q=0)} = \frac{1}{2} \left[\frac{1}{P} \begin{pmatrix} P \\ k \end{pmatrix} \pm N_{\text{palindrom}} \right] \quad (21)$$

symmetric and antisymmetric eigenvectors, respectively.

In the non-zero momentum subspaces ($q \neq 0$), the consequences of the reflection symmetry (17) are less stringent. Clearly, (17) implies that one may select eigenvectors of the decay coefficient matrices $R(q)$ that share the symmetry (17). Similar to the reasoning above, the interchangeability of symmetrization using the matrix S , and the reflection operation R ensures that the eigenvectors $U(q)$ of the symmetrized Hermitian matrix $\tilde{R}(q)$ [eq. (38), diagonalization script] can be chosen to obey:

$$U_3(q) = \pm U_{[RE\bar{z}]}(q)^* \quad (22)$$

for symmetric and antisymmetric configurations, respectively.

the additional symmetry under reflection further simplifies the problem.

We have already seen that all eigenstates of the diffusion problem, possibly after proper symmetrization, are also eigenstates of the reflection operator R (see Section (b)). Now, an (anti-)symmetric state fulfills:

$$\langle [z|v] \rangle = \pm \langle [R[z]|p-v] \rangle \quad (16)$$

In the momentum representation, this leads to the symmetry property:

$$\begin{aligned} \langle (z|q) \rangle &= \frac{1}{p} \sum_{v=0}^{p-1} e^{-2\pi i q v / p} \langle [z|v] \rangle \\ &= \pm \frac{1}{p} \sum_{v=0}^{p-1} e^{-2\pi i q v / p} \langle [R[z]|p-v] \rangle \\ &= \pm \frac{1}{p} \sum_{v=0}^{p-1} e^{2\pi i q v / p} \langle [R[z]|v] \rangle \\ &= \pm \langle (R[z]|q) \rangle^* \end{aligned} \quad (17)$$

This has various consequences. We start out with the subspace of zero momentum ($q=0$). In this case, $\langle (z|0) \rangle$ is a real quantity, and therefore:

$$\langle (z|0) \rangle = \frac{1}{p} \sum_{v=0}^{p-1} \langle [z|v] \rangle = \pm \langle (R[z]|0) \rangle \quad (18)$$

It follows from (18) that in the symmetric eigenvectors, the elements connected to z and $R[z]$ have the same value, whereas they are of opposed sign for antisymmetric eigenvectors. Then, in particular, all components representing palindromic primitives $z = R[z]$ vanish.

In fact, we may rewrite (18) in the form:

$$\left\langle \frac{1}{2} \{ (z|0) \mp (R[z]|0) \} \right\rangle = 0 \quad (19)$$

Therefore, introducing symmetric and antisymmetric base states in the $q=0$ momentum subspace:

These eigenvectors then form the unitary transformation matrix $U(q)$ in (41) [diagonalization script]. However, the orthonormal base set of eigenvectors composing the transformation matrix is not uniquely defined, even if all eigenvalues λ of $R(q)$ are distinct (nondegenerate case). Indeed, the conditions:

$$R(q) \vec{u}(q) = \lambda \vec{u}(q), \quad \vec{u}(q)^+ \vec{u}(q) = 1, \quad \vec{u}(q)^+ \vec{v}(q) = 0 \quad (23)$$

(where $\vec{u}(q)$, $\vec{v}(q)$ denote different eigenvectors) still leave the opportunity to assign a random unitary phase $e^{i\varphi}$ to each eigenvector:

$$\vec{u}(q) \rightarrow e^{i\varphi} \vec{u}(q) \quad (24)$$

These arbitrary phases show up in numerical diagonalization. Here, however, we may take advantage of them in order to resolve the sign ambiguity in (22). Multiplying all anti-symmetric eigenvectors $\vec{u}_{(A)}(q)$ in (22) by the special phase factor $i = \exp[i\pi/2]$, while leaving the symmetric subset $\vec{u}_{(S)}(q)$ unchanged, yields:

$$\begin{aligned} i \vec{u}_3^{(A)}(q) &= -i \vec{u}_{R[3]}^{(A)}(q)^* = \{i \vec{u}_{R[3]}^{(A)}(q)\}^* \\ \vec{u}_3^{(S)}(q) &= \vec{u}_{R[3]}^{(S)}(q)^* \end{aligned} \quad (25)$$

so that it is always possible to select an orthonormal set of eigenvectors $\vec{u}(q)$ of $R(q)$ with the property:

$$\vec{u}_3(q) = \vec{u}_{R[3]}(q)^* \quad (26)$$

In this representation, the elements of the eigenvectors $\vec{u}_3(q)$ pertaining to palindromic configurations ($z = R[z]$) are always real, while the entries for pairs of mirror image primitives are conjugate complex. If the real part of such an element is stored at the position of z , and the imaginary part stored at the position of $R[z]$ (where, say, $z \in R[z]$ in their binary representation, see page 7, diagonalization script), the unitary matrix $U(q)$ can be stored in a real-number array of size $N_{\text{prim}} \times N_{\text{prim}}$, resulting in considerable savings of computer memory.