The Diffusion Problem: Eigenvalues in Simple Diffusion

(a) Evolution of single-site averages

In simple diffusion, the rate of a jump event does not depend on the occupation status of the sites adjacent to the sites involved in the jump: Whenever a jump event is possible, i.e., the site neighbouring the atom is empty, it will take place at a constant rate A.

Next, consider the evolution of the average occupation of a single site ν, i.e., of the average $\langle\bullet\rangle_\nu$. According to the general ideas put forward in the script on diagonalization [Section (d)], the change of occupation is due to loss to neighbouring empty sites, and the gain from adjacent occupied sites through jumps to site ν. All configurations that contribute to the loss thus contain the pattern $\cdots\underset{\nu+1}{\circ}\underset{\nu}{\bullet}\cdots$ (for clockwise jumps) or $\cdots\underset{\nu}{\bullet}\underset{\nu-1}{\circ}\cdots$ (for counter-clockwise jumps). Similarly, the gain terms stem from the patterns $\cdots\underset{\nu+1}{\bullet}\underset{\nu}{\circ}\cdots$ (clockwise jump) and $\cdots\underset{\nu}{\circ}\underset{\nu-1}{\bullet}\cdots$ (counterclockwise jump). The rates do not depend on the sites not specified here.

Hence, after summation over all configurations $[\zeta|\nu]$ matching these patterns, we obtain a differential equation for the evolution of $\langle\bullet\rangle_\nu$:

$$\frac{d}{dt}\langle\underset{\nu}{\bullet}\rangle = -A\left(\langle\underset{\nu+1}{\circ}\underset{\nu}{\bullet}\rangle + \langle\underset{\nu}{\bullet}\underset{\nu-1}{\circ}\rangle\right) + A\left(\langle\underset{\nu+1}{\bullet}\underset{\nu}{\circ}\rangle + \langle\underset{\nu}{\circ}\underset{\nu-1}{\bullet}\rangle\right) \qquad (1)$$

Now, by conservation of probability, $\langle\underset{\nu+1}{\bullet}\underset{\nu}{\bullet}\rangle + \langle\underset{\nu+1}{\circ}\underset{\nu}{\bullet}\rangle = \langle\underset{\nu}{\bullet}\rangle$ must hold (the site $\nu+1$ is either occupied or empty, after all), and in the same fashion, $\langle\underset{\nu+1}{\bullet}\underset{\nu}{\bullet}\rangle + \langle\underset{\nu+1}{\bullet}\underset{\nu}{\circ}\rangle = \langle\underset{\nu+1}{\bullet}\rangle$. An analogous relation holds for the averages containing site $\nu-1$, and we may use them to eliminate the particle-hole correlators in (1). Then, we find that also the two-particle averages cancel, and one is left with:

$$\frac{d}{dt}\langle\underset{\nu}{\bullet}\rangle = A\left(\langle\underset{\nu+1}{\bullet}\rangle - 2\langle\underset{\nu}{\bullet}\rangle + \langle\underset{\nu-1}{\bullet}\rangle\right) \qquad (2)$$

(We note in passing that this reasoning fails if jump rates depend on the status of neighbouring sites, i.e., if not all jump rates A, B, C, D are equal. Cancellation then does no longer take place.)

Eq. (2) is similar in structure to the original master equation (17) (see diagonalization script). In particular, the translational invariance implicit in (2) allows to decouple the differential equation in momentum space. We introduce the momentum state averages $\langle q \rangle$ analogously to (18), (19):

$$\langle q \rangle = \frac{1}{p} \sum_{\nu=0}^{p-1} e^{-2\pi i q \nu / p} \langle \underset{\nu}{\bullet} \rangle$$

$$\langle \underset{\nu}{\bullet} \rangle = \sum_{q=0}^{p-1} e^{2\pi i q \nu / p} \langle q \rangle \qquad (3)$$

After performing the summation over sites in (2), the diffusion equation for $\langle q \rangle$ becomes:

$$\frac{d}{dt} \langle q \rangle = A \left(e^{-2\pi i q/p} - 2 + e^{2\pi i q/p} \right) \langle q \rangle$$

$$= -2A \left(1 - \cos \frac{2\pi q}{p} \right) \langle q \rangle$$

$$= -4A \sin^2 \frac{\pi q}{p} \cdot \langle q \rangle \qquad (4)$$

This is completely identical to the diffusion of a single atom ($k=1$) on a circle of p sites, as comparison to Section (h), script on diagonalization, shows: Unstable wave-like modes $\langle q \rangle$ of the single-site averages decay exponentially with a time constant $\lambda_q = -4A \sin^2 \frac{\pi q}{p}$: $\langle q \rangle(t) = \langle q \rangle(t_0) \exp[-\lambda_q (t - t_0)]$.

Now, alternatively we may evaluate the master equation (25) for the complete k-atom problem in momentum space, and then form a proper trace over the solution vector $\vec{\rho}(q,t)$ (26) (see the script on diagonalization, Section (f)).

For simplicity, we start out with an eigenstate $\vec{\rho}_\alpha(Q)$ in the subspace with momentum Q, where:

$$R(Q) \vec{\rho}_\alpha(Q) = \lambda_\alpha \vec{\rho}_\alpha(Q) \qquad (5)$$

According to (25) [diagonalization script], this state decays exponentially with the time constant λ_α, and consequently all averages obtained from this "pure" state will follow the same decay law. In configuration space, $\vec{\rho}_\alpha(Q)$ corresponds to a wavelike superposition of configurations [d.s., (19)]:

$$[\mathfrak{z}|\nu]_\alpha = e^{2\pi i Q\nu/p}\,(\mathfrak{z}|Q)_\alpha \tag{6}$$

where $(\mathfrak{z}|Q)_\alpha$ is the component of $\vec{\rho}_\alpha(Q)$ assigned to the primitive $\mathfrak{z}$. The corresponding site average $\langle \underset{\mu}{\bullet} \rangle$ in the state $\vec{\rho}_\alpha(Q)$ is obtained after summation over all matching patterns $[\mathfrak{z}|\nu]_\alpha$ in (6):

$$\langle \underset{\mu}{\bullet} \rangle = \sum_{\mathfrak{z}} (\mathfrak{z}|Q)_\alpha \cdot \sum_{\nu=0}^{p-1} e^{2\pi i Q\nu/p}\,\Theta\big[[\mathfrak{z}|\nu],\mu\big] \tag{7}$$

where $\Theta\big[[\mathfrak{z}|\nu],\mu\big] = 1$ for matching patterns, i.e., the μth site in $[\mathfrak{z}|\nu]$ is occupied, and otherwise $\Theta\big[[\mathfrak{z}|\nu],\mu\big] = 0$. Since $[\mathfrak{z}|\nu]$ and $[\mathfrak{z}|0]$ are arrangements that are merely rotated to each other by ν sites, the relation:

$$\Theta\big[[\mathfrak{z}|\nu],\mu\big] = \Theta\big[[\mathfrak{z}|0],\mu-\nu\big] \tag{8}$$

follows at once. From (7), we calculate the momentum-space average $\langle q \rangle$ (3) for the pure state $\vec{\rho}_\alpha(Q)$:

$$\begin{aligned}\langle q \rangle &= \frac{1}{p}\sum_{\mu=0}^{p-1} e^{-2\pi i q\mu/p}\,\langle \underset{\mu}{\bullet} \rangle \\ &= \frac{1}{p}\sum_{\mathfrak{z}} (\mathfrak{z}|Q)_\alpha \cdot \sum_{\nu=0}^{p-1}\sum_{\mu=0}^{p-1} e^{2\pi i (Q\nu - q\mu)/p}\,\Theta\big[[\mathfrak{z}|\nu],\mu\big]\end{aligned} \tag{9}$$

Using (8), one of the sums in (9) can be evaluated in closed form. Introduce $\beta = \mu - \nu$ as new summation index that, in modulo p arithmetic, again covers the interval $0, 1, \ldots, p-1$:

$$\begin{aligned}&\sum_{\nu=0}^{p-1}\sum_{\mu=0}^{p-1} e^{2\pi i (Q\nu - q\mu)/p}\,\Theta\big[[\mathfrak{z}|\nu],\mu\big] = \\ &= \sum_{\beta=0}^{p-1} e^{-2\pi i q\beta/p}\,\Theta\big[[\mathfrak{z}|0],\beta\big] \cdot \sum_{\nu=0}^{p-1} e^{2\pi i (Q-q)\nu/p} \\ &= p\cdot \delta_{Q,q \bmod p} \sum_{\beta=0}^{p-1} e^{-2\pi i q\beta/p}\,\Theta\big[[\mathfrak{z}|0],\beta\big]\end{aligned} \tag{10}$$

(The geometric series vanishes unless $(Q-q)_{\bmod p} = 0$.) After insertion in (9), one then finds:

$$\langle q\rangle = \delta_{Q,q \bmod p} \sum_{z} \left(\sum_{\beta=0}^{p-1} e^{2\pi i q\beta/p}\, \Theta[[z|0],\beta]\right)^* (z|Q)_\alpha \tag{11}$$

As expected, the average $\langle q\rangle$ is limited to the same momentum subspace $q=Q$ as the pure state. The interesting new result in (11) is now that the right-hand side decays like $\exp[\lambda_\alpha(t-t_0)]$, whereas $\langle Q\rangle$ has the decay constant $\lambda_Q = -4A\sin^2(\pi Q/p)$ (4).

If we introduce a vector $\vec{u}_Q$ whose elements are given by the sums in (10), (11):

$$u_Q[z] = \sum_{\beta=0}^{p-1} e^{2\pi i Q\beta/p}\, \Theta[[z|0],\beta] \tag{12}$$

this means that the sum over primitives z in (11) must vanish unless the left-hand and right-hand eigenvalues are identical:

$$\sum_{z} u_Q[z]^* (z|Q)_\alpha = \vec{u}_Q^{\,+}\cdot\vec{\rho}_\alpha(Q) = 0 \quad \text{if } \lambda_Q \neq \lambda_\alpha, \tag{13}$$

i.e., the vectors $\vec{u}_Q$ and $\vec{\rho}_\alpha(Q)$ are then orthogonal. Since it is easily verified that $\vec{u}_Q$ does not vanish, and there is a complete orthonormal base set of eigenvectors $\vec{\rho}_\alpha(Q)$ ($\alpha = 1, 2, \ldots, N_{prim}$) for the hermitian matrix $R(Q)$ [$R(Q)$ is always hermitian for $B=C$, see eq. (32), diagonalization script], there must be at least one eigenvalue λ_α of $R(Q)$ for which:

$$\lambda_\alpha = \lambda_Q = -4A\sin^2\frac{\pi Q}{p} \tag{14}$$

and the vector $\vec{u}_Q$ (12) must itself be an eigenvector of $R(Q)$ with eigenvalue λ_Q. We verified the first part of this statement for the special case $p=5$, $k=2$ in the course of a laborious calculation [see Section (i), diagonalization script, eqs. (75)-(80).]

Finally, we determine the norm of the vectors $\vec{u}_Q$, as this allows to find the normalized eigenvector $\vec{\rho}_Q$ that must appear in the unitary transformation matrix $U(Q)$ diagonalizing $R(Q)$ [see (33), diagonalization script]. This enterprise yields some valuable insights into the nature of these special eigenvectors.

We first examine the rather trivial case $Q=0$. Then, $\lambda_Q = 0$ follows from (14), and $\vec{\rho}_0$ must be the unitary equilibrium eigenvector $\vec{\rho}_{eq}$ of the system which for $B=C$ is composed from equal entries:

$$\rho_{eq}[z] = \frac{1}{\sqrt{N_{prim}}} = \sqrt{\frac{k!(p-k)!}{(p-1)!}} \tag{15}$$

[see (2), diagonalization script]. Clearly, for $Q=0$ the summation in (12) merely yields the number of atoms k:

$$u_0[z] = \sum_{\beta=0}^{p-1} \Theta[[z|0],\beta] = k \tag{16}$$

and hence $\|\vec{u}_0\|^2 = N_{prim} \cdot k^2$:

$$\rho_{eq}[z] = \frac{1}{k\sqrt{N_{prim}}}\, u_0[z] = \frac{1}{\sqrt{N_{prim}}} \tag{17}$$

In the next step, we show that the sum over the square norms of the whole set of eigenvectors $\|\vec{u}_Q\|^2$, $Q=0,1,2,\dots,p-1$, is also quite easy to obtain. From (12), this sum is:

$$\begin{aligned}
\sum_{Q=0}^{p-1} \|\vec{u}_Q\|^2 &= \sum_z \sum_{Q=0}^{p-1} |u_Q[z]|^2 \\
&= \sum_z \sum_{\beta=0}^{p-1} \sum_{\beta'=0}^{p-1} \sum_{Q=0}^{p-1} e^{2\pi i Q(\beta-\beta')/p}\, \Theta[[z|0],\beta]\, \Theta[[z|0],\beta'] \\
&= \sum_z \sum_{\beta=0}^{p-1} \sum_{\beta'=0}^{p-1} p \cdot \delta_{\beta,\beta' \bmod p}\, \Theta[[z|0],\beta]\, \Theta[[z|0],\beta'] \\
&= p \cdot \sum_z \sum_{\beta=0}^{p-1} \Theta[[z|0],\beta]^2 \\
&= p \cdot \sum_z \sum_{\beta=0}^{p-1} \Theta[[z|0],\beta] = p \cdot k \cdot N_{prim}
\end{aligned} \tag{18}$$

Here, we first used the fact that the geometrical Q series vanishes unless $\beta = \beta' \pmod p$, that $\Theta[\dots]$ only takes the values 0 and 1 and thus $\Theta[\dots]^2 = \Theta[\dots]$ must hold, and finally (16).

In the concluding step, we finally establish that the vectors $\vec{u}_Q$ for non-zero momentum $Q=1,2,\dots,p-1$ differ merely in the sequence of their elements, i.e., are actually permutations of each other, and therefore share the same norm $\|\vec{u}_Q\|^2$ (which is, however, different from $\|\vec{u}_0\|^2$ – see above).

To this end, we introduce a special set of permutations among the primitive patterns $\mathfrak{z}$ that we will call the powers $\mathfrak{z}^j$ $(j=1,2,\dots,p-1)$ of the primitive. Their definition is fairly simple: If $\nu_1, \nu_2, \dots, \nu_k$ is the set of sites occupied in the primitive $\mathfrak{z}$, then the occupied sites in $\mathfrak{z}^j$ are given by:

$$(j\nu_1)_{\mathrm{mod}\,p},\ (j\nu_2)_{\mathrm{mod}\,p},\ \dots,\ (j\nu_k)_{\mathrm{mod}\,p} \tag{19}$$

As the pattern sum $r = \nu_1+\nu_2+\dots+\nu_k = 0$ by definition vanishes in a primitive pattern (see diagonalization script, pg. 6), the same holds true for the powers $\mathfrak{z}^j$:

$$r(j) = \left[j\nu_1 + j\nu_2 + \dots + j\nu_k\right]_{\mathrm{mod}\,p} = (j\cdot r)_{\mathrm{mod}\,p} = 0 \tag{20}$$

i.e., the patterns $\mathfrak{z}^j$ are themselves primitive. It is straightforward to establish that the index j indeed behaves like the exponent of a conventional number:

$$(\mathfrak{z}^j)^{j'} = (\mathfrak{z}^{j'})^j = \mathfrak{z}^{(j\cdot j')_{\mathrm{mod}\,p}} \tag{21}$$

In particular, for every $j=1,2,\dots,p-1$ there exists exactly one "inverse" j^{-1} so that $(j\cdot j^{-1})_{\mathrm{mod}\,p} = 1$ (see eq. (5),(6) in the diagonalization script). Since:

$$(\mathfrak{z}^j)^{j^{-1}} = \mathfrak{z} \tag{22}$$

for every primitive $\mathfrak{z}$, there must be a one-to-one correspondence between the sets $\{\mathfrak{z}\}$ and $\{\mathfrak{z}^j\}$, and the assignment between $\mathfrak{z}$ and $\mathfrak{z}^j$ must be bijective. In other words, the power operation performs a permutation within the set of primitives.

For $j = p-1 = -1_{\mathrm{mod}\,p}$, atoms at site ν are replaced with atoms at the mirror image site $(p-\nu)_{\mathrm{mod}\,p}$. The "inverse" $\mathfrak{z}^{-1}$ of a primitive therefore is its image under reflection:

$$\mathfrak{z}^{p-1} = \mathfrak{z}^{-1} = \mathbb{R}[\mathfrak{z}] \tag{23}$$

The reflection operation $\mathbb{R}$ thus is a special member of the class of power permutations.

As a simple example, consider the case $p=5$, $k=2$ covered in detail in Section (i), diagonalization script. There are only two primitives, ○●●○○ (sites $v_1=2$, $v_2=3$ occupied, binary code 12) and ●○○●○ (sites $v_1=1$, $v_2=4$ occupied, binary code 18), and their permutation table under the power operation is:

$z \backslash j$	z^1	z^2	z^3	z^4
(12)	○●●○○	●○○●○	●○○●○	○●●○○
(18)	●○○●○	○●●○○	○●●○○	●○○●○

Note that $z = z^4 = z^{-1}$ (both patterns are palindromic) and $z^2 = z^{-2} = z^3$; squaring z exchanges both patterns, however.

The relevance of the power operation in this context is the following property of the matching operator $\Theta[[z|0],\beta]$ (8):

$$\Theta[[z|0],\beta] = \Theta[[z^j|0],(j\beta)_{\mathrm{mod}\,p}] \tag{24}$$

that results directly from the definition of z^j (19). Inserting this relation into the representation of the eigenvector $\vec{u}_Q$ (12), we find:

$$\begin{aligned} u_Q[z] &= \sum_{\beta=0}^{p-1} e^{2\pi i Q\beta/p}\,\Theta[[z|0],\beta] \\ &= \sum_{\beta=0}^{p-1} e^{2\pi i (Q\beta)_{\mathrm{mod}\,p}/p}\,\Theta[[z^Q|0],(Q\beta)_{\mathrm{mod}\,p}] \\ &= \sum_{\beta'=0}^{p-1} e^{2\pi i \beta'/p}\,\Theta[[z^Q|0],\beta'] = u_1[z^Q] \end{aligned} \tag{25}$$

(Note that with β, also the product $\beta' = (Q\beta)_{\mathrm{mod}\,p}$ will cover the entire set $\beta' = 0,1,2,\dots,p-1$, since there is an inverse to the factor Q. We already used this reasoning above.) Consequently, the elements $u_Q[z]$ and $u_1[z^Q]$ are identical, and the components of these eigenvectors [and for that purpose, all eigenvectors $\vec{u}_1$, $\vec{u}_2, \dots, \vec{u}_{p-1}$ of the respective decay coefficient matrices $R(1), R(2), \dots, R(p-1)$] are merely permuted in sequence.

Since with z also z^Q covers the entire set of primitives, all vectors $\vec{u}_Q$ share the same square norm:

$$\|\vec{u}_Q\|^2 = \sum_{\mathfrak{z}} |u_Q[\mathfrak{z}]|^2 = \sum_{\mathfrak{z}^Q} |u_1[\mathfrak{z}^Q]|^2 = \|\vec{u}_1\|^2 \qquad (26)$$

The norm itself is easily established using the sum over all eigenvector norms (18), and the previously found value for $q=0$, $\|\vec{u}_0\|^2 = k^2 \cdot N_{prim}$:

$$\|\vec{u}_Q\|^2 = \frac{1}{p-1}\left(\sum_{q=0}^{p-1} \|\vec{u}_q\|^2 - \|\vec{u}_0\|^2\right) \qquad (Q \neq 0)$$

$$= \frac{k(p-k)}{p-1} N_{prim}$$

$$= \frac{k(p-k)}{p(p-1)} \binom{p}{k} = \binom{p-2}{k-1} = \frac{(p-2)!}{(k-1)!(p-k-1)!} \qquad (27)$$

Properly normalized eigenvectors $\vec{\rho}_Q$ of the decay rate matrices in momentum space $R(Q)$ are thus given by $(Q \neq 0)$:

$$\rho_Q[\mathfrak{z}] = \frac{1}{\sqrt{\binom{p-2}{k-1}}} \sum_{\beta=0}^{p-1} e^{2\pi i Q\beta/p}\, \Theta\big[[\mathfrak{z}|0], \beta\big] \qquad (28)$$

and their respective eigenvalues are $\lambda_Q = -4A \sin^2 \frac{\pi Q}{p}$ (14).

(b) <u>Degeneracy of eigenvalues in the $q=0$ subspace</u>

We have already seen that in the subspace of zero momentum $(q=0)$, reflection symmetry enforces that always a complete base of eigenvectors $\vec{u}_\nu(q=0)$, $\nu = 1, 2, \ldots, N_{prim}$ of the decay coefficient matrix $R(0)$ exists that possesses definite symmetry with respect to the reflection operation $\mathbb{R}$:

$$R(0)\,\vec{u}_\nu(0) = \lambda_\nu(0)\,\vec{u}_\nu(0), \qquad \mathbb{R}\,\vec{u}_\nu(0) = \pm\,\vec{u}_\nu(0) \qquad (29)$$

[see the script on reflection properties, Section (d)]. According to eq. (21) in this script, the number of symmetric and antisymmetric eigenstates N_{symm}, N_{anti} is given by:

$$N^{(q=0)}_{\substack{symm\\anti}} = \frac{1}{2}\left[\frac{1}{p}\binom{p}{k} \pm \binom{(p-1)/2}{z}\right] \qquad (30)$$

respectively, where $z = k/2$ for k even, and $z = (k-1)/2$ for odd k [see eqs. (14) and (15) there.]

These results are valid for arbitrary choices of the jump rates A, B, C, D. A much stronger statement apparently holds in the case of simple diffusion ($A = B = C = D$) and is the subject of the following conjecture:

Conjecture. If $A = B = C = D$, the spectrum of the decay matrix in zero momentum subspace $R(0)$ is degenerate and consists of:

(i) $N_{palindrom}$ isolated eigenvalues λ_μ with eigenvectors $\vec{u}_\mu(0)$ that are symmetric under reflection,

(ii) $N_{anti}^{(q=0)}$ distinct eigenvalues λ_ν whose eigenspaces are all two-fold degenerate and of indefinite symmetry, i.e. for these λ_ν, both a symmetric and antisymmetric eigenvector $\vec{u}_\nu^{(S)}(0)$, $\vec{u}_\nu^{(A)}(0)$ are available.

While a proof of this conjecture is not readily available, the conjecture has been shown to hold in numerous examples. In a heuristic interpretation, each palindromic primitive $\mathfrak{z} = \mathbb{R}[\mathfrak{z}]$ seems to "generate" an isolated symmetric eigenstate, while each mirror image pair $\eta = \mathbb{R}[\mathfrak{z}]$, $\mathfrak{z} = \mathbb{R}[\eta]$ gives rise to an eigenvalue with twofold degeneracy and mixed symmetry. There is, however, no indication of a direct assignment between primitives and eigenvalues.

A remarkable consequence of the conjecture is the existence of "conjugation operators" $\mathbb{C}$ that transform symmetric into anti-symmetric eigenstates, while leaving the evolution of the system invariant. This means if the vector $\vec{\rho}(0,t)$ in eq (25), diagonalization script, is a solution of the master equation:

$$\frac{d}{dt}\vec{\rho}(0,t) = R(0)\vec{\rho}(0,t) \tag{31}$$

then the same property holds for the conjugated image vector:

$$\frac{d}{dt}\left[\mathbb{C}\vec{\rho}(0,t)\right] = R(0)\left[\mathbb{C}\vec{\rho}(t,0)\right] \tag{32}$$

Clearly, this requires that $\mathbb{C}$ and $R(0)$ commute:

$$R(0)\,\mathbb{C} = \mathbb{C}\cdot R(0) \tag{33}$$

Since the jump rates do not distinguish between the clockwise and counterclockwise directions, the same property holds under mirror reflection (see also eq. (3), reflection script):

$$R(0)\,\mathbb{R} = \mathbb{R}\cdot R(0) \tag{34}$$

Finally, in order to exchange the symmetry property of the solution, reflection $\mathbb{R}$ and conjugation operator $\mathbb{C}$ must anticommute:

$$\mathbb{R}\mathbb{C} + \mathbb{C}\mathbb{R} = 0 \tag{35}$$

Then, an eigenvector $\vec{u}$ of $\mathbb{R}$, with $\mathbb{R}\vec{u} = \rho\vec{u}$, will be transformed into an eigenvector $\mathbb{C}\vec{u}$ of opposite symmetry $-\rho$:

$$\mathbb{R}\left[\mathbb{C}\vec{u}\right] = -\mathbb{C}\mathbb{R}\vec{u} = -\rho\cdot\mathbb{C}\vec{u} \tag{36}$$

while eigenvectors of $R(0)$ with eigenvalue λ are transformed into eigenvectors with the same eigenvalue:

$$R(0)\left[\mathbb{C}\vec{u}\right] = \mathbb{C}\cdot R(0)\,\vec{u} = \lambda\cdot\mathbb{C}\vec{u} \tag{37}$$

By combination of (36) and (37), we find that $\mathbb{C}$ must annihilate all eigenvectors $\vec{u}_\mu(0)$ with nondegenerate eigenvalues λ_μ: $\mathbb{C}\vec{u}_\mu = \vec{0}$. Hence, all conjugation operators are singular.

If one assumes the conjecture to hold, it is fairly straightforward to construct classes of operators of type $\mathbb{C}$. To this end, we note that we can then arrange the eigenvalues λ of $R(0)$ as a sequence of pairs λ_ν (for the degenerate eigenspaces), followed by the sequence of $N_{\text{palindrom}}$ isolated eigenvalues λ_μ. Furthermore, we may selected an orthonormal set of basis vectors $\vec{u}_\nu, \vec{u}_\mu$ with definite symmetry under reflection, so that for each degenerate eigenvalue λ_ν

the first eigenvector $\vec{u}_\nu^{(S)}$ is symmetric, $\mathbb{R}\vec{u}_\nu^{(S)} = \vec{u}_\nu^{(S)}$, and the second eigenvector $\vec{u}_\nu^{(A)}$ is antisymmetric under reflection, $\mathbb{R}\vec{u}_\nu^{(A)} = -\vec{u}_\nu^{(A)}$. These eigenvectors then form the columns of the orthogonal transformation matrix $\mathcal{U}(0)$ diagonalizing the decay coefficient matrix $R(0)$ [see the script on diagonalization, eq. (33)]:

$$R(0) = \mathcal{U}(0)\,\Lambda(0)\,\mathcal{U}(0)^T \tag{38}$$

whereby:

$$\Lambda(0) = \begin{pmatrix} \lambda_1\epsilon & & & & 0 \\ & \ddots & & & \\ & & \lambda_\nu\epsilon & & \\ & & & \lambda_1^{(P)} & \\ 0 & & & & \lambda_\mu^{(P)} \ddots \end{pmatrix}, \tag{39}$$

$$\mathcal{U}(0) = \left(\vec{u}_1^{(S)}, \vec{u}_1^{(A)}, \vec{u}_2^{(S)}, \vec{u}_2^{(A)}, \ldots, \vec{u}_\nu^{(S)}, \vec{u}_\nu^{(A)}, \ldots, \vec{u}_1^{(P)}, \ldots, \vec{u}_\mu^{(P)}, \ldots\right)$$

Here, $\epsilon = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ is the 2x2 unit matrix, and $\lambda_\mu^{(P)}$, $\vec{u}_\mu^{(P)}$ denote isolated eigenvalues with their symmetric eigenvectors.

Since all eigenvectors $\vec{u}_\nu^{(S)}$, $\vec{u}_\mu^{(P)}$ are invariant under $\mathbb{R}$, whereas $\vec{u}_\nu^{(A)}$ changes its sign, the orthogonal matrix $\mathcal{U}(0)$ diagonalizes $\mathbb{R}$ as well:

$$\mathbb{R} = \mathcal{U}(0)\,\rho\,\mathcal{U}(0)^T \tag{40}$$

where:

$$\rho = \begin{pmatrix} \sigma_z & & & & & 0 \\ & \sigma_z & & & & \\ & & \ddots & & & \\ & & & \sigma_z & & \\ & & & & 1 & \\ 0 & & & & & 1 \ddots \end{pmatrix} \tag{41}$$

Here, the Pauli matrices $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ replace the unit matrices ϵ in (39). As both ρ and $\Lambda(0)$ are diagonal, these matrices commute and therefore:

$$R(0)\,\mathbb{R} = \mathcal{U}(0)\,\Lambda(0)\,\rho\,\mathcal{U}(0)^T = \mathcal{U}(0)\,\rho\,\Lambda(0)\,\mathcal{U}(0)^+ = \mathbb{R}\,R(0) \tag{42}$$

as demanded by (34). (Note that $\mathcal{U}(0)^T\mathcal{U}(0) = \mathbb{1}$.)

It is now simple to construct hermitian matrices $\mathbb{C}$ by similiarity transforms employing $\mathcal{U}(0)$:

$$\mathbb{C} = \mathcal{U}(0)\,\gamma\,\mathcal{U}(0)^T \tag{43}$$

For the relation (33) to hold, $\Lambda(0)$ (39) and γ must commute: $\Lambda(0)\gamma = \gamma\Lambda(0)$. This implies that γ is block-diagonal and consists of (2×2)-matrices C_ν along the diagonal that trivially commute with the corresponding entries $\lambda_\nu E$, whereas the part representing the nondegenerate eigenvalues $\lambda_\mu^{(p)}$ in $\Lambda(0)$ will commute only with a diagonal matrix $(c_1, \ldots, c_\mu, \ldots)$. Anticommutation (35) enforces that γ must also obey $\gamma P = -P\gamma$, which in view of (41) requires the two relations:

$$\begin{aligned} C_\nu\sigma_z + \sigma_z C_\nu &= 0 \\ c_\mu\cdot 1 + 1\cdot c_\mu = 2c_\mu &= 0 \end{aligned} \tag{44}$$

for the degenerate and nondegenerate subspaces, respectively. The second relation is fulfilled only by $c_\mu \equiv 0$, while by basic spin algebra, the solution of the first condition is an arbitrary linear combination of the Pauli matrices $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ and $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$:

$$C_\nu = \alpha_\nu\sigma_x + \beta_\nu\sigma_y \tag{45}$$

where α_ν, β_ν are real coefficients:

$$\gamma = \begin{pmatrix} \alpha_1\sigma_x + \beta_1\sigma_y & & & & 0 \\ & \ddots & & & \\ & & \alpha_\nu\sigma_x + \beta_\nu\sigma_y & & \\ & & & \ddots\; 0 & \\ 0 & & & & \ddots\; 0 \ldots \end{pmatrix} \tag{46}$$

The matrix γ is thus always singular, but not uniquely determined. Clearly, the hope is that for a certain choice of parameters, $\mathbb{C}$ takes on a simple form that provides information about the hidden symmetry that causes the multiple degeneracy of $\mathcal{R}(0)$.

Alternatively (and equivalently), special matrices $\mathbb{C}_\nu$ with the desired properties (33) and (35) can be constructed from the symmetric and antisymmetric normalized eigenvectors $\vec{u}_\nu^{(S)}, \vec{u}_\nu^{(A)}$ in the degenerate subspace of $R(0)$ with eigenvalue λ_ν. For this purpose, we form the outer or tensorial product:

$$\mathbb{C}_\nu = \vec{u}_\nu^{(S)} \otimes \vec{u}_\nu^{(A)T} + \vec{u}_\nu^{(A)} \otimes \vec{u}_\nu^{(S)T} \tag{47}$$

(In practical terms, this means that the matrix element $\mathbb{C}_\nu[\eta, \zeta]$ is given by:

$$\mathbb{C}_\nu[\eta, \zeta] = u_\nu^{(S)}[\eta]\, u_\nu^{(A)}[\zeta] + u_\nu^{(A)}[\eta]\, u_\nu^{(S)}[\zeta]\,.) \tag{48}$$

Since $R(0)\, \vec{u}_\nu^{(S,A)} = \lambda_\nu \vec{u}_\nu^{(S,A)}$ for both eigenvectors, one finds:

$$R(0)\, \mathbb{C}_\nu = \lambda \mathbb{C}_\nu = \mathbb{C}_\nu R(0) \tag{49}$$

i.e., (33), and correspondingly:

$$\begin{aligned} \mathbb{R}\mathbb{C}_\nu &= \vec{u}_\nu^{(S)} \otimes \vec{u}_\nu^{(A)T} - \vec{u}_\nu^{(A)} \otimes \vec{u}_\nu^{(S)T} \\ \mathbb{C}_\nu \mathbb{R} &= -\vec{u}_\nu^{(S)} \otimes \vec{u}_\nu^{(A)T} + \vec{u}_\nu^{(A)} \otimes \vec{u}_\nu^{(S)T} \end{aligned} \tag{50}$$

or $\mathbb{R}\mathbb{C}_\nu + \mathbb{C}_\nu \mathbb{R} = 0$, as demanded by (35). The form (47) is obtained from the general solution (46) by setting all coefficients α, β to zero, except $\alpha_\nu = 1$.

In any numerical evaluation of the eigenvectors, the degeneracy of the eigenspaces generally leads to eigenvectors $\vec{u}_\nu^{(1,2)}$ of no definite symmetry, i.e., two orthonormal linear combinations of the symmetric and antisymmetric base vectors $\vec{u}_\nu^{(S)}, \vec{u}_\nu^{(A)}$. They must be related to the basis set of definite symmetry through a rotation (only an orthogonal transform will preserve the norm and orthogonality of the vectors), possibly combined with a reflection:

$$\begin{pmatrix} \vec{u}_\nu^{(1)} \\ \vec{u}_\nu^{(2)} \end{pmatrix} = \begin{pmatrix} \cos\Theta_\nu & -\sin\Theta_\nu \\ \sin\Theta_\nu & \cos\Theta_\nu \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & \pm 1 \end{pmatrix} \begin{pmatrix} \vec{u}_\nu^{(S)} \\ \vec{u}_\nu^{(A)} \end{pmatrix} \tag{51}$$

Eigenstates of the reflection operator $\mathbb{R}$ can be extracted from the numerically determined pair of eigenvectors $\vec{u}_\nu^{(1)}, \vec{u}_\nu^{(2)}$ either by simple projection and subsequent normalization [see the script on reflection, eq. (7)]:

$$\vec{u}_\nu^{(S)} = \frac{\mathbb{P}_S \vec{u}_\nu^{(1)}}{\|\mathbb{P}_S \vec{u}_\nu^{(1)}\|^{1/2}} , \quad \vec{u}_\nu^{(A)} = \frac{\mathbb{P}_A \vec{u}_\nu^{(1)}}{\|\mathbb{P}_A \vec{u}_\nu^{(1)}\|^{1/2}} \tag{52}$$

where either $\vec{u}_\nu^{(1)}, \vec{u}_\nu^{(2)}$, or any linear combination of them may serve as the initial state that undergoes projection. Alternatively, one may employ the orthogonal transformation (51) directly. Since:

$$\mathbb{P}_S \vec{u}_\nu^{(1)} = \cos\Theta_\nu \cdot \vec{u}_\nu^{(S)} , \quad \mathbb{P}_S \vec{u}_\nu^{(2)} = \sin\Theta_\nu \cdot \vec{u}_\nu^{(S)} \tag{53}$$

we find with the projector property $\mathbb{P}_S^2 = \mathbb{P}_S$:

$$\begin{aligned} \cos 2\Theta_\nu &= \cos^2\Theta_\nu - \sin^2\Theta_\nu = \|\mathbb{P}_S \vec{u}_\nu^{(1)}\|^2 - \|\mathbb{P}_S \vec{u}_\nu^{(2)}\|^2 \\ \sin 2\Theta_\nu &= 2\sin\Theta_\nu \cos\Theta_\nu = 2\, \vec{u}_\nu^{(2)T} \cdot \mathbb{P}_S \cdot \vec{u}_\nu^{(1)} \end{aligned} \tag{54}$$

and therefore for the rotation angle in (51):

$$\tan 2\Theta_\nu = \frac{2\, \vec{u}_\nu^{(2)T} \cdot \mathbb{P}_S \cdot \vec{u}_\nu^{(1)}}{\|\mathbb{P}_S \vec{u}_\nu^{(1)}\|^2 - \|\mathbb{P}_S \vec{u}_\nu^{(2)}\|^2} \tag{55}$$

While being slightly more complicated, the method of rotation has the advantage to be unconditionally stable in a numerical sense.

(c) Example: Three particles on seven sites

We now illustrate these developments using the simplest model that includes all the features discussed above, viz., simple diffusion of $k=3$ atoms on a circular arrangement of $p=7$ sites. In the first step, we identify the $N_{prim} = \frac{6!}{3!4!} = 5$ different primitive patterns of the system. They are listed in the following table, together with their binary codes:

6	5	4	3	2	1	0			
○	○	●	○	●	●	○	=	(22)	
○	○	●	●	○	○	●	=	(25)	
○	●	○	○	●	○	●	=	(37)	(56)
●	○	○	○	○	●	●	=	(67)	
●	●	○	●	○	○	○	=	(104)	

It is easily verified that (25), (37), and (67) represent palindromic patterns invariant under mirror reflection, whereas the primitives (22) and (104) are mirror images of each other.

For the eigenstates $\vec{\rho}_Q$ (28) relevant in the diffusive evolution of one-site averages $\langle \bullet \rangle$ discussed in Section (a), also the permutations under the power operation (19) are of interest. The powers of the primitives z listed in (57) are assembled below:

z	z^2	z^3	z^4	z^5	z^6
(22)	(22)	(104)	(22)	(104)	(104)
(25)	(67)	(37)	(37)	(67)	(25)
(37)	(25)	(67)	(67)	(25)	(37)
(67)	(37)	(25)	(25)	(37)	(67)
(104)	(104)	(22)	(104)	(22)	(22)

(57)

(Note that $z^6 = R[z]$.) The permutations form two separate groups, one involving the three palindromic patterns, the other one the mirror image pair (22), (104).

The elements of the special eigenvectors $\vec{\rho}_Q$ of $R(Q)$ are given by (28):

$$\rho_Q[z] = \frac{1}{\sqrt{10}} \sum_{\beta=0}^{6} e^{2\pi i Q\beta/7}\, \Theta[[z|0],\beta] \tag{58}$$

Since $\rho_Q[z] = \rho_1[z^Q]$ (25), it suffices to calculate the elements $\rho_1[z]$ of the vector in the momentum subspace $Q=1$; the components of the other vectors are easily looked up in table (57).

In order to express the result in compact form, it is useful to insert a brief mathematical interlude. In a fashion somewhat similar to the methods used in Section (i), diagonalization script, we examine relations between seventh roots of unity:

One starts with the observation that these roots add up to zero:

$$\sum_{\beta=0}^{6} e^{2\pi i\beta/7} = 0 \tag{59}$$

as summation of the geometric series shows. Using (59), one verifies at once by expansion into exponentials:

$$\cos\frac{2\pi}{7} + \cos\frac{4\pi}{7} + \cos\frac{6\pi}{7} = -\frac{1}{2}, \tag{60}$$

$$\cos\frac{2\pi}{7}\cos\frac{4\pi}{7} + \cos\frac{4\pi}{7}\cos\frac{6\pi}{7} + \cos\frac{6\pi}{7}\cos\frac{2\pi}{7} = -\frac{1}{2}, \tag{61}$$

$$\cos\frac{2\pi}{7}\cos\frac{4\pi}{7}\cos\frac{6\pi}{7} = \frac{1}{8} \tag{62}$$

from which one obtains a cubic equation:

$$\left(z-\cos\frac{2\pi}{7}\right)\left(z-\cos\frac{4\pi}{7}\right)\left(z-\cos\frac{6\pi}{7}\right) = z^3 + \frac{z^2}{2} - \frac{z}{2} + \frac{1}{8} \tag{63}$$

that possesses the three roots $\cos\frac{2\pi}{7}$, $\cos\frac{4\pi}{7}$, $\cos\frac{6\pi}{7}$, which are therefore algebraic numbers. From (60), one finds:

$$\left|e^{2\pi i/7} + e^{4\pi i/7} + e^{8\pi i/7}\right|^2 = 3 + 2\left(\cos\frac{2\pi}{7} + \cos\frac{4\pi}{7} + \cos\frac{6\pi}{7}\right) = 2 \tag{64}$$

which, together with $\cos\frac{6\pi}{7} = \cos\frac{8\pi}{7}$, yields:

$$\mathrm{Re}\left[e^{2\pi i/7} + e^{4\pi i/7} + e^{8\pi i/7}\right] = \cos\frac{2\pi}{7} + \cos\frac{4\pi}{7} + \cos\frac{6\pi}{7} = -\frac{1}{2}, \tag{65}$$

$$\mathrm{Im}\left[e^{2\pi i/7} + e^{4\pi i/7} + e^{8\pi i/7}\right] = \sqrt{|\ldots|^2 - \mathrm{Re}[\ldots]^2} = \frac{\sqrt{7}}{2} \tag{66},$$

or:

$$e^{2\pi i/7} + e^{4\pi i/7} + e^{8\pi i/7} = -\frac{1}{2} + \frac{\sqrt{7}}{2}i \tag{67}$$

These results are relevant for the eigenvector in (58) that now reads explicitly using the atomic positions listed in (56):

$$\vec{\gamma}_1 = \frac{1}{\sqrt{10}}\begin{pmatrix} e^{2\pi i/7} + e^{4\pi i/7} + e^{8\pi i/7} \\ 1 + e^{6\pi i/7} + e^{8\pi i/7} \\ 1 + e^{4\pi i/7} + e^{10\pi i/7} \\ 1 + e^{2\pi i/7} + e^{12\pi i/7} \\ e^{6\pi i/7} + e^{10\pi i/7} + e^{12\pi i/7} \end{pmatrix} = \frac{1}{\sqrt{10}}\begin{pmatrix} -\frac{1}{2} + \frac{\sqrt{7}}{2}i \\ 1 + 2\cos\frac{6\pi}{7} \\ 1 + 2\cos\frac{4\pi}{7} \\ 1 + 2\cos\frac{2\pi}{7} \\ -\frac{1}{2} - \frac{\sqrt{7}}{2}i \end{pmatrix} \tag{68}$$

Its eigenvalue is $\lambda_1 = -4A\sin^2\frac{\pi}{7}$ (14). Using the relations (60) and (61), it is rather easy to verify that $\vec{\rho}_1$ is indeed of unit length, as postulated by (27). As noted above, the other special eigenvectors $\vec{\rho}_Q$ follow from (68) by permutation.

In passing, we remark that the elements in $\vec{\rho}_1$ pertaining to palindromic primitives are all real, while the mirror image pair (22), (104) gives rise to conjugate complex entries. This is in accordance with the general observations made in Section (a), script on reflection properties [cf. eq. (26)].

Next, we turn our attention to the decay coefficient matrix $R(0)$ in the zero momentum subspace. Analyzing all possible jumps between the arrangements in (56) one finds that transitions between all primitives are possible, with the exception of jumps between the compact arrangement (67) and the primitives (25) and (37). (The latter jumps would violate the selection rule $|\Delta m| \leq 1$ for the number of blocks, see the script on diagonalization.) Properly weighed, the coefficient decay matrix becomes:

$$R(0) = A \begin{pmatrix} -4 & 1 & 1 & 1 & 1 \\ 1 & -4 & 2 & 0 & 1 \\ 1 & 2 & -4 & 0 & 1 \\ 1 & 0 & 0 & -2 & 1 \\ 1 & 1 & 1 & 1 & -4 \end{pmatrix} \qquad (69)$$

Since $A=B=C=D$, the matrix is symmetric, and may be diagonalized in the form (38). Its eigenvalues are remarkably simple; the characteristic polynomial of $R(0)$:

$$\left[\lambda^5 + 18A\cdot\lambda^4 + 117A^2\lambda^3 + 320A^3\lambda^2 + 300A^4\lambda\right] = \\ = \lambda(\lambda+2A)(\lambda+5A)^2(\lambda+6A) \qquad (70)$$

allows for complete factorization with negative integer multiples of the rate A as eigenvalues. In accordance with the conjecture stated in Section (b), $R(0)$ possesses three isolated eigenvalues $\lambda_1^{(P)}=0$, $\lambda_2^{(P)}=-2A$, $\lambda_3^{(P)}=-6A$, supposedly related to the three palindromic patterns (25), (37), (67), and a doubly degenerate eigenvalue $\lambda=-5A$ somehow linked to the pair of images under reflection (22), (104).

Using their orthonormality property, it is rather straightforward to determine a set of eigenvectors $\vec{\rho}_\nu$ of $R(0)$ (69) correspon-ding to these eigenvalues that furthermore show definite symmetry under reflections $\mathbb{R}$. Apart from the choice of sign, these eigen-vectors are unique. The symmetric and antisymmetric eigen-vectors of unit norm in the degenerate eigenspace $\lambda = -5A$ read:

$$\vec{u}^{(S)} = \frac{1}{\sqrt{30}}\begin{pmatrix} 3 \\ -2 \\ -2 \\ -2 \\ 3 \end{pmatrix}, \qquad \vec{u}^{(A)} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ -1 \end{pmatrix}, \tag{71}$$

whereas the symmetric eigenvectors for the isolated eigenvalues $\lambda_1^{(P)} = 0$, $\lambda_2^{(P)} = -2A$, $\lambda_3^{(P)} = -6A$ are found as:

$$\vec{u}_1^{(P)} = \frac{1}{\sqrt{5}}\begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \quad \vec{u}_2^{(P)} = \frac{1}{\sqrt{6}}\begin{pmatrix} 0 \\ 1 \\ 1 \\ -2 \\ 0 \end{pmatrix}, \quad \vec{u}_3^{(P)} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \\ 0 \end{pmatrix}, \tag{72}$$

respectively. These eigenvectors form the columns of the orthogonal transformation matrix $\mathcal{U}(0)$ in (39):

$$\mathcal{U}(0) = \left[\vec{u}^{(S)}, \vec{u}^{(A)}, \vec{u}_1^{(P)}, \vec{u}_2^{(P)}, \vec{u}_3^{(P)}\right] \tag{73}$$

and according to (39) – (41), one obtains the decompositions:

$$R(0) = A\begin{pmatrix} -4 & 1 & 1 & 1 & 1 \\ 1 & -4 & 2 & 0 & 1 \\ 1 & 2 & -4 & 0 & 1 \\ 1 & 0 & 0 & -2 & 1 \\ 1 & 1 & 1 & 1 & -4 \end{pmatrix} = \mathcal{U}(0)\begin{pmatrix} -5A & 0 & 0 & 0 & 0 \\ 0 & -5A & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2A & 0 \\ 0 & 0 & 0 & 0 & -6A \end{pmatrix}\mathcal{U}(0)^T \tag{74}$$

$$\mathbb{R} = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix} = \mathcal{U}(0)\cdot\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}\cdot\mathcal{U}(0)^T \tag{75}$$

Since there is only a single mirror image pair (22), (104) among the primitives in this problem, the operator $\mathbb{C}$ that transforms the symmetric vector $\vec{u}^{(S)}$ in the degenerate subspace into the antisymmetric basis vector $\vec{u}^{(A)}$ (71) and vice versa is uniquely defined. From (46), (47), it is seen that:

$$\mathbb{C} = \mathcal{U}(0)\begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}\mathcal{U}(0)^T = \vec{u}^{(s)} \otimes \vec{u}^{(A)T} + \vec{u}^{(A)} \otimes \vec{u}^{(s)T} \tag{76}$$

The explicit form of $\mathbb{C}$ then follows from (48), (71):

$$\mathbb{C} = \frac{1}{\sqrt{15}}\begin{pmatrix} 3 & -1 & -1 & -1 & 0 \\ -1 & 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 1 & -3 \end{pmatrix} \tag{77}$$

It is easily verified that indeed $\mathbb{C}\vec{u}^{(s)} = \vec{u}^{(A)}$, $\mathbb{C}\vec{u}^{(A)} = \vec{u}^{(s)}$, $\mathbb{C}\vec{u}^{(P)} = \vec{0}$, $R(0)\mathbb{C} = \mathbb{C}R(0) = -5A\,\mathbb{C}$ (49), and $\mathbb{C}\mathbb{R} = -\mathbb{R}\mathbb{C}$ (50) hold, and that the hermitian $\mathbb{C}$ thus transforms symmetric solutions $\vec{\rho}^{(s)}(0,t)$ of the master equation (31) into antisymmetric solutions $\vec{\rho}^{(A)}(0,t)$ and vice versa. The physical reason behind the existence of the symmetry-breaking operator $\mathbb{C}$ (77) at this point remains obscure, however.