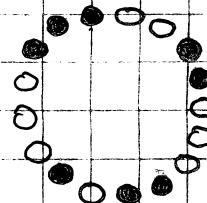


The Diffusion Problem: The Diagonalization Scheme

(a) Jumps and their properties

Consider an arrangement of k atoms on p sites that are arranged in a circular fashion. (Later on, it will prove practical to choose a prime number of sites.) We mark occupied sites by ● and empty sites by ○.



Example: $k=8, p=17$.

In a jump event, an atom may leave its site and instantaneously occupy one of its two neighbouring sites, provided they are empty. Depending on the state of the sites surrounding the location of the jump, these events occur with one of four different frequencies (jump rates):

(i) Type A: Motion of an isolated atom

This jump occurs if the immediately adjacent sites of both the initial and final location of the atom are empty. Both before and after the jump, the atom possesses no immediate neighbours. Schematically:

... ○ ● ○ ○ ... or ... ○ ○ ○ ○ ...

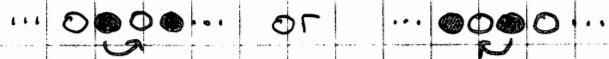
(ii) Type B: Separation of an atom from a block

This type designates jumps that involve atoms that possess initially a direct neighbour, but lose it during the event. Schematically:

... ● ○ ○ ○ ... or ... ○ ○ ○ ○ ...

(iii) Type C: Fusion of an atom to a block

The rate applies to jumps of atoms that initially have no neighbouring occupied site, but possess a neighbouring atom once the jump is performed. Schematically:



(iv) Type D: Exchange of an atom between blocks

These jumps concern the case that the moving atom has a neighbouring occupied site both before and after the event. Schematically:



Note that the rates do not depend on the direction of the jump (clockwise or counterclockwise). The jumps preserve the symmetry of the atomic configuration under mirror reflections.

The list of jumps A,B,C,D (i)-(iv) exhausts the different configurations with respect to the occupation of next neighbors. Interactions with second-next neighbouring sites are not included. In the special case of equal rates $A=B=C=D$, also the dependence on next neighbours cancels out and simple diffusion, only guided by the availability of sites, prevails.

Relation between jumps and inverse jumps: By definition, the inverse jump to a given jump is one that restores the original configuration. It is easily seen that the types of jumps are related according to this table:

Original jump:	A	B	C	D
Inverse jump:	A	C	B	D

Jumps of type A and D have inverses of the same type, while jumps of type B and C exchange their role. Note that original and inverse jumps obviously point into opposite directions.

The relation outlined above is reflected in the evolution of the "block number" m under jumps. This quantity details the number of contiguous (uninterrupted) stretches of atoms on the circle. (In the figure, $m=4$.) The block number is a key quantity in the determination of the equilibrium properties of the system (see separate script.) Clearly, the change Δm in the block number as a function of the jump type is:

jump type:	A	B	C	D
change Δm :	0	+1	-1	0

Elementary jumps with $|\Delta m| > 1$ never occur.

Atom-hole symmetry: Every jump of an atom may equivalently viewed as the jump of a hole, as illustrated below:

$$\text{atomic jump } \cdots \circ \circ \bullet \cdots \equiv \text{hole jump } \cdots \bullet \circ \circ \cdots$$

(Note that the direction is reversed, but this does not influence the jump rates.) However, the type assignment of the jump does depend on whether a hole or an atom is considered the moving agent:

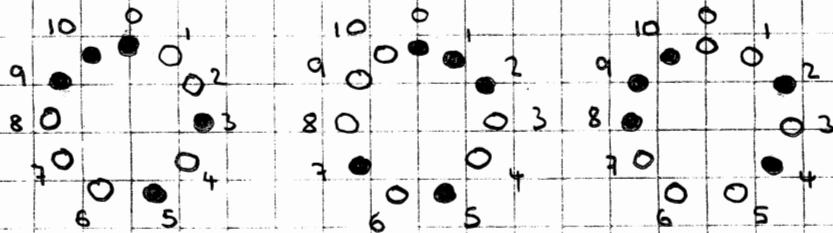
atom jump	isolated	separation	fusion	exchange
hole jump	exchange	separation	fusion	isolated

i.e., an atom jump of type A is a hole jump of type D and vice versa, whereas jumps of type B and C retain their character independent of the choice of atoms or holes. In essence, this means that the evolution of a system of k atoms on p sites, and the evolution of a system of k holes [$p-k$ atoms] on p sites are identical, once the rates for jumps of type A and D are exchanged, and atom and holes interchange their roles.

(b) The classification of patterns

We consider two arrangements of k atoms on p sites as congruent, if a simple rotation of the entire pattern will transform them into each other. The properties of these patterns are necessarily related - for example, they have identical equilibrium occupation probabilities, etc.

To be concise, we pick one of the p sites as the "origin" and label it with 0; the remainder of the sites are labelled 1, 2, 3, etc., $p-2, p-1$, in a clockwise sense. Obviously, since the sites form a closed loop, and $p-1$ is the left neighbour to site 0, such a scheme defines the number of a site only up to multiples of the site number p , and we have to use modulo arithmetic throughout.



The figure shows three congruent arrangements of $k=5$ atoms on $p=11$ sites that differ only in their state of rotation. We may say that these states are equivalent (unlike arrangements that cannot be transformed into each other by simple rotations), and it suffices to select a single member of each set of equivalent states (each equivalence class) as a representant.

We thus need a scheme to distinguish the members in each set and pick a representative member. In a simple approach, we form the pattern sum r , the sum over the designations of all occupied sites. In the example above:

$$\begin{aligned} r_1 &= [0 + 3 + 5 + 9 + 10] \bmod 11 = 5 \bmod 11 \\ r_2 &= [0 + 1 + 2 + 5 + 7] \bmod 11 = 4 \bmod 11 \\ r_3 &= [2 + 4 + 8 + 9 + 10] \bmod 11 = 0 \bmod 11 \end{aligned}$$

(Note that we again use the addition modulo p .)

The pattern sums all differ. It is easy to see that in general, a clockwise rotation of a pattern by ℓ sites will change the pattern sum r by an amount:

$$r' - r = [\ell \cdot k] \bmod p \quad (1)$$

We note that the right-hand side of (1) will become zero only if $\ell \cdot k$ is a multiple of p ; if we choose the number of sites to be prime, (1) will never be zero, except if ℓ itself is a multiple of p . But then, $\ell \bmod p = 0$, the rotation is trivial, and the patterns are identical. Thus, two different congruent patterns show different pattern sums. On the other hand, for prime p , every equivalence class also contains a member with given pattern sum $r = 0, 1, 2, \dots, p-1$. (To verify this statement, take a pattern and rotate it by $\ell = 0, 1, 2, \dots, p-1$ sites. If any two of these patterns, say \mathbf{r} and \mathbf{r}' , had identical pattern sums, we would find from (1) that $[(\ell - \ell') \cdot k] \bmod p = 0$, which implies $(\ell - \ell')$ is a divisor of p , and hence a multiple of p — $\ell = \ell'$ follows.)

To summarize: If the number of sites p is prime, then the p patterns that emerge from rotation of a given pattern by $0, 1, 2, \dots, p-1$ sites possess different pattern sums r_0, r_1, \dots, r_{p-1} and are therefore all distinct. Conversely, for each given pattern and fixed pattern sum there exists a rotation ℓ so that the rotated pattern will show the desired pattern sum. There is a one-to-one correspondence between pattern sums and rotational states of the same pattern.

(The strong assertions fail if the number of sites is not prime, but composite. E.g., for $p=4$ and $k=2$ the equivalence class of the pattern $\bullet\bullet$ contains four states linked through rotations:

$$\begin{array}{ccccccc} \bullet & \bullet & & \circ & \bullet & & \bullet & \bullet \\ & & & & & & & \\ \circ & \circ & & \circ & \bullet & & \bullet & \circ \end{array}$$

but the pattern $\circ\circ$ only contains two members in its class:

$$\begin{array}{ccccc} \bullet & \circ & \circ & \bullet & \\ & & & & \\ \circ & \bullet & & \bullet & \circ \end{array}$$

The corresponding pattern sums $r=1, 3, 1, 3$ and $r=2, 0$ are also

(6)

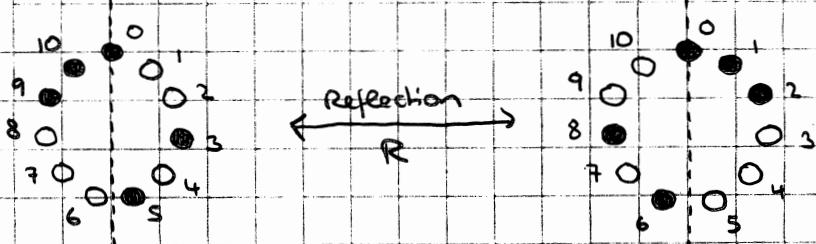
not unique.)

A simple way to pick individual representatives from the congruent sets of arrangements now consists in selecting patterns with given pattern sum r . We make the simple choice $r=0$ and call the resulting patterns primitive. For each equivalence class, with p members, there is exactly one primitive. In the figure on page 4, the rightmost pattern is the primitive representative of the set.

Number of primitives: Each primitive represents p possible, distinct arrangements. Since there are $\binom{p}{k}$ combinations to select k sites out of p and occupy them with atoms, the number of primitives N_{prim} is:

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

Reflection of patterns: A comprehensive analysis of the behaviour of patterns under reflection is the topic of a separate script. Here, we briefly define the reflection operation. We pick the site 0 as the fixed element of the reflection, and otherwise swap the contents of the sites k and $p-k$:

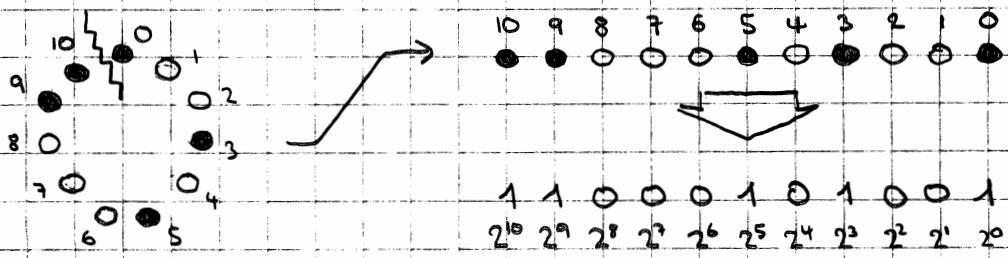


Consequently, the pattern sum changes under reflections as:

$$\begin{aligned} r' &= [(p-v_1) + (p-v_2) + \dots + (p-v_k)] \bmod p \\ &= [kp - (v_1 + v_2 + \dots + v_k)] \bmod p \\ &= -r \bmod p \end{aligned} \quad (3)$$

Therefore, for a primitive pattern we find $r' = r = 0$: Under reflections, primitive patterns transform into primitive patterns.

Sorting of patterns : Once the origin of a pattern is fixed, it is easy to establish an ordering relation between the arrangements. For this purpose, open the circle of sites between $p-1$ and 0 , stretch it, and replace every occupied site by "1" and every empty site by "0":



The final string of p digits is interpreted as a binary number. Obviously, this scheme accommodates every arbitrary combination of atoms and holes on p sites, and any two arrangements can be unambiguously ordered by their associated numbers.

Selection of patterns : The correspondence between patterns and binary numbers suggests a simple selection scheme :

- (i) Examine the binary representation of every ordinal between 0 and $2^p - 1$ for the number of "1" digits. This is the number of atoms in the corresponding pattern. If this number does not equal k , discard the pattern, otherwise;
- (ii) Form the pattern sum r by summing over the positions of the "1" digits in the binary representation; if it is not a multiple of p , discard; otherwise
- (iii) add to the list of primitive patterns.

This algorithm will produce a complete ordered list of the primitive patterns. However, step (i) is not efficient, since the number of combinations to be examined grows exponentially with p , while for fixed k the number of primitives $N_{\text{prim}}(k)$ is only a polynomial function of p . It is therefore advisable to replace (i) by a slightly more sophisticated algorithm that covers all combinations with k atoms:

(a) Start out with a "rightmost" combination of atoms:

10	9	8	7	6	5	4	3	2	1	0
0	0	0	0	0	0	•	•	•	•	•

(β) In each step, shift the rightmost atom for which this is possible one site to the left, then assemble all atoms to the right of the jumping atom in the rightmost position:

10	9	8	7	6	5	4	3	2	1	0
0	0	0	•	0	•	•	•	0	0	•

10	9	8	7	6	5	4	3	2	1	0
0	0	0	•	0	0	0	0	0	0	•

(γ) This scheme stops once the "leftmost" configuration is reached:

10	9	8	7	6	5	4	3	2	1	0
•	•	•	•	•	0	0	0	0	0	0

Since the associated binary number in step (β) steadily increases, the output is an ordered list. Induction shows that it is also complete.

The numerical correspondence allows to specify any given configuration of atoms by two numbers — one designating the primitive pattern of its equivalence class, the other one its shift v , i.e., its relative state of rotation with respect to this primitive pattern. To be specific, v is the number of sites that the primitive pattern has to be rotated clockwise in order to obtain the desired arrangement. (As an example, in the figure of page 4, the rightmost pattern is primitive ($v=0$), while the congruent left and center patterns show shift numbers $v=1$ and $v=3$, respectively.) We label such a pattern in the form:

[primitive | v] (4)

The pattern sum of such a state will obviously be given by:

$$r = [v \cdot k]_{\text{mod } p} \quad (5)$$

[cf. eq. (1)]. Since there is a unique correspondence between the pattern sum r and the shift number v , we may invert the relation (5) and express v through r :

$$v = [r/k] \bmod p \quad (6)$$

(9)

where the "modulo division" implies that v/k is r plus a multiple of the site number p . (There is no easy way of calculating (6), except testing all $v=1, 2, \dots, p-1$.)

The relation (6) becomes important when examining the effects of the individual jump events introduced in Section (i). Depending on the direction of the jump (clockwise or counterclockwise), a single atom will change to a neighbouring site, and the pattern sum will be altered in the process:

$$\begin{aligned} \Delta r &= +1 && (\text{clockwise}) \\ \Delta r &= -1 && (\text{counterclockwise}) \end{aligned} \quad (7)$$

The corresponding changes in the shifts v follow from (5) and (6). If we write $r' = r + \Delta r = r \pm 1$, and $v' = v + \Delta v$, we find from (5):

$$r + \Delta r = [(v + \Delta v), k] \bmod p = r + [\Delta v \cdot k] \bmod p \quad (8)$$

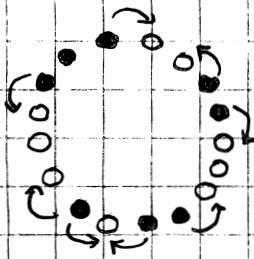
or $[\Delta v \cdot k] \bmod p = 1$; this shows that the change of the shift variable is a constant whose sign depends on the direction of the jump:

$$\begin{aligned} \Delta v &= [1/k] \bmod p && (\text{clockwise}) \\ \Delta v &= -[1/k] \bmod p && (\text{counterclockwise}) \end{aligned} \quad (9)$$

Note that the actual value of this constant depends on k and p in a non-intuitive fashion.

(c) The combinatorics of jumps

In an intermission, we briefly evaluate the numbers of essentially different jump events that can occur between the rotational equivalence classes. We already established that there are $\frac{1}{p} \binom{p}{k}$ primitive patterns with k atoms on p sites; from the figures, it is clear that jumps can occur only at the boundary of contiguous atomic blocks:



The rightmost member of every block may jump in clockwise sense, the leftmost in counterclockwise direction. If m is the number of blocks in the primitive, there are hence m different possible events in each direction. The total number of jumps is then given by summation over all primitives; denote the number of primitives with m blocks by $N(p,k,m)$, we find successively:

$$\begin{aligned}
 N_p &= \sum_m m N(p,k,m) \\
 &= \sum_m \frac{(k-1)}{m-1} \frac{(p-k-1)}{m-1} = \sum_m \frac{1}{(m-1)!} \frac{(1-k)_{m-1} (1+k-p)_{m-1}}{(1)_{m-1}} \\
 &= {}_2F_1(1-k, 1+k-p, 1; 1) \\
 &= \frac{\Gamma(1) \Gamma(p-1)}{\Gamma(k) \Gamma(p-k)} = \frac{(p-2)!}{(k-1)! (p-k-1)!} = \binom{p-2}{k-1} \quad (10)
 \end{aligned}$$

(Here, we successively used the closed form for $N(p,k,m)$ (7), the representation of the sum through Pochhammer symbols $(a)_n$, the summation into a hypergeometric function, and its special value for unit argument. For details, see the script on equilibrium properties of the diffusion problem, and Abramowitz/Stegun, Handbook of mathematical functions, Chapter 15.)

It follows that $N_p = N_G$ is equal to the number of different possibilities to place $k-1$ atoms on $p-2$ sites. This result may be interpreted in this fashion: To ensure the feasibility of a clockwise jump, a pattern must contain the combination $\bullet\circ$. Once we fix the atom-hole combination at the sites 0 and 1, there are (by simple combinatorics) $\binom{p-2}{k-1}$ different arrangements of k atoms on p sites. These arrangements are in general

not primitive, but they are related to a primitive by rotation. Every primitive will contain m members of its equivalence class in the set of arrangements, because there is a rotational state for each block to end at position 0 that contributes to the set. Hence, both methods actually count the same set, and must deliver an identical result.

The equivalence of the approaches furthermore allows to illuminate the number of the different jump types in each direction. (By symmetry, the numbers must be the same in either direction.) We stay here with clockwise jumps.

To generate a jump of type A, the atom in question must be isolated before and after the event. This fixes a four-site sequence [see section (a)]:

$\dots \bullet \bullet \bullet \bullet \dots$

Following the reasoning above, the number of different events of "A" type among all primitives is the number of ways to occupy the remaining $p-4$ sites with the $k-1$ leftover atoms:

$$N_p(A) = \binom{p-4}{k-1} \quad (11)$$

Similarly, "B" type events require the four-site subsequence $\dots \bullet \bullet \bullet \bullet \dots$, and "C" type jumps occur in the sequence $\dots \bullet \bullet \bullet \bullet \dots$. Both require the presence of two atoms, leaving $k-2$ atoms to be distributed among the remaining sites:

$$N_p(B) = N_p(C) = \binom{p-4}{k-2} \quad (12)$$

Note that $N_p(B) = N_p(C)$ follows. Finally, "D" type jumps describe the exchange of an atom between blocks: $\dots \bullet \bullet \bullet \bullet \dots$, and thus occur:

$$N_p(D) = \binom{p-4}{k-3} \quad (13)$$

times. It is trivial to check that the sum of (11) - (13) indeed yields the total number of clockwise jumps $N_p(10)$.

We finally note that the m configurations generated by the various clockwise jumps in a primitive pattern of block number m are essentially different, i.e., the resulting patterns are all incongruent and belong to distinct equivalence classes, represented by primitives of their own. To see this, we note that the configurations resulting from the jumps will differ (since different atoms have been moved) in order to be equivalent, and represented by the same primitive, they necessarily must possess different rotational shifts ν in their representation (4). But according to (9), the change in shift $\Delta\nu$ caused by a clockwise jump is constant: $\Delta\nu = [1/k]_{\text{mod}p}$. Hence, the resulting patterns must belong to different equivalence classes. In summary:

To each primitive z_m with block number m , there are:

- exactly m distinct primitives η_f related to z_m via clockwise jumps,
- exactly m distinct primitives η_b related to z_m via counterclockwise jumps.

Note that the same primitive η_f may show up in both the forward and backward jump groups, and one of the resulting primitives may actually be identical to the original pattern z_m . The type of the jumps is closely linked to the accompanying change of the block number Δm , see Section (a).

(d) Diffusion: The master equation

The occupation probability of any given state [primitive $z|\nu$] (4) evolves over time due to jumps into neighbouring states, as detailed in Section (i). Let us denote the rates of individual jumps of types A-D by the same symbols A, B, C, D; for simplicity, we represent the transition rates from the equivalence class of the primitive pattern z to the equivalence class of the primitive η_f for (counter) clockwise jumps by:

(13)

$$R_D(\eta, z), R_G(\eta, z)$$

(14)

According to the line of reasoning above, for given $z = z_m$ there are exactly m primitives η_D, η_G for which $R_D(\eta, z)$ and $R_G(\eta, z)$ are nonzero, respectively; in this case the rate is either A, B, C, or D, depending on the type of jump. Note that the table on page 2 translates into the following symmetry relation for the jump coefficient matrices R_D, R_G :

$R_D(\eta, z)$	0	A	B	C	D
$R_G(z, \eta)$	0	A	C	B	D

(15)

i.e., they are symmetric under exchange of the rates B, C, and exchange of the sense of rotation.

The master equation contains two parts, the loss of probability of a given configuration due to jumps into different configurations, and the gain through the reverse jumps from these arrangements. The first term is represented by the total jump rate $R(\eta)$:

$$R(\eta) = \sum_z [R_D(z, \eta) + R_G(z, \eta)] \quad (16)$$

The total temporal evolution of the occupation of the state $[\eta | v]$ is then governed by the equation:

$$\begin{aligned} \frac{d}{dt} \langle [\eta | v] \rangle &= -R(\eta) \langle [\eta | v] \rangle + \\ &+ \sum_z R_D(\eta, z) \langle [z | v - \Delta v] \rangle \\ &+ \sum_z R_G(\eta, z) \langle [z | v + \Delta v] \rangle \end{aligned} \quad (17)$$

where $\Delta v = [1/k]_{\text{mod}} p$ (9). Here, we used the fact that a clockwise jump causes a shift Δv in the rotation number required to reduce the pattern to its primitive counterpart.

(e) The momentum representation

In equation (17), terms with different shift v are coupled, but the relative distances $\pm \Delta v$ of the terms involved do not actually depend on v . This property expresses the rotational

(14)

invariance of the system. It also allows to decouple the system of equations (17) by the use of momentum states.

By definition, a momentum state $(\bar{z}|q)$ is connected to the rotational states $[\bar{z}|v]$ via the discrete Fourier transform:

$$(\bar{z}|q) = \frac{1}{P} \sum_{v=0}^{P-1} e^{-2\pi i q v / P} [\bar{z}|v] \quad (18)$$

where q is allowed to take any of the numbers $0, 1, 2, \dots, P-1$. Apart from the prefactor, this transformation is unitary, and its inverse transformation reads:

$$[\bar{z}|v] = \sum_{q=0}^{P-1} e^{2\pi i q v / P} (\bar{z}|q) \quad (19)$$

(For a proof, multiply the transformation matrices, and evaluate the ensuing geometrical series!)

$$\frac{1}{P} \sum_{q=0}^{P-1} e^{2\pi i q \mu / P} e^{-2\pi i q v / P} = \delta(\mu \bmod P, v \bmod P) \quad (20)$$

which vanishes unless $(\mu - v) \bmod P = 0$.)

Using (18) to sum over all rotational shifts v in (17), one obtains the master equation in momentum space:

$$\begin{aligned} \frac{d}{dt} \langle (\eta|q) \rangle &= -R(\eta) \langle (\eta|q) \rangle \\ &+ \sum_{\bar{z}} R_D(\eta, \bar{z}) \cdot \frac{1}{P} \sum_{v=0}^{P-1} e^{-2\pi i q v / P} \langle [\bar{z}|v - \Delta v] \rangle \\ &+ \sum_{\bar{z}} R_G(\eta, \bar{z}) \cdot \frac{1}{P} \sum_{v=0}^{P-1} e^{-2\pi i q v / P} \langle [\bar{z}|v + \Delta v] \rangle \end{aligned} \quad (21)$$

Shifting the index of summation in (21) by $\mp \Delta v$, we infer that the sums indeed describe the momentum state $(\bar{z}|q)$, albeit with prefactors $\exp(\mp 2\pi i q \Delta v / P)$, i.e. conjugate complex P th roots of unity. Defining the rate coefficient matrix $R(\eta, \bar{z}; q)$ via:

$$\begin{aligned} R(\eta, \bar{z}; q) &= -R(\eta) \delta_{\eta, \bar{z}} + \\ &+ e^{-2\pi i q \Delta v / P} R_D(\eta, \bar{z}) + e^{2\pi i q \Delta v / P} R_G(\eta, \bar{z}) \end{aligned} \quad (22)$$

One finds that the equations in (21) are decoupled into a set of p master equations for each momentum value q : (15)

$$\frac{d}{dt} \langle (\gamma_1 q) \rangle = \sum_z R(\gamma_1 z; q) \langle (z|q) \rangle \quad (23)$$

As discussed in section (c), the matrices $R(\gamma_1 z; q)$, which share common non-zero elements, become sparse with increasing number of primitives N_{prim} (2), (10).

Since all coefficients $R_2(\gamma_1 z)$, $R_6(\gamma_1 z)$ are real, we furthermore note that:

$$R(\gamma_1 z; p-q) = R(\gamma_1 z; q)^*, \quad (24)$$

i.e. the rate coefficient matrices for the momenta q and $-q \bmod p$ are conjugate complex. In particular, the matrix $R(\gamma_1 z; q=0)$ is real.

(f) Solution of the master equation

Assembling the state averages $\langle (z|q) \rangle$ into probability vectors $\vec{p}(q)$, and denoting the rate coefficient matrix by $R(q)$, the system (23) can be formally written as a set of p matrix equations:

$$\frac{d}{dt} \vec{p}(q, t) = R(q) \vec{p}(q, t) \quad (q=0, 1, 2, \dots, p) \quad (25)$$

where $\vec{p}(q)$ is a vector of dimension N_{prim} (2), of which $(p+1)/2$ have to be solved numerically. (The solution of the remaining $(p-1)/2$ equations follows trivially from the symmetry relation (24) — with $\vec{p}(q, t)$ is also $\vec{p}(-q, t)^*$ a solution.) Since $R(q)$ does not depend on the time parameter t , (25) is formally solved by integration:

$$\vec{p}(q, t) = \exp[R(q)(t-t_0)] \vec{p}(q, t_0) \quad (26)$$

To actually perform the matrix exponentiation, the eigen-vectors and eigenvalues of $R(q)$ must be determined, in general in a numerical fashion. Assembling the eigenvalues

in a diagonal matrix $\Lambda(q)$ and the corresponding eigenvectors column-by-column into the transformation matrix $D(q)$, we find:

$$R(q) = D(q) \Lambda(q) D(q)^{-1}, \quad (27)$$

i.e., $R(q)$ and $\Lambda(q)$ are similar matrices, and by expanding the exponential into a series,

$$\begin{aligned} \exp[R(q)t] &= \mathbb{1} + R(q) + \frac{1}{2!} R(q)^2 + \dots \\ &= D(q) \left[\mathbb{1} + \Lambda(q) + \frac{1}{2!} \Lambda(q)^2 + \dots \right] D(q)^{-1} \\ &= D(q) \exp[\Lambda(q)t] D(q)^{-1} \end{aligned} \quad (28)$$

The exponential of a diagonal matrix, however, is again diagonal, and its elements are the exponentials of the original elements.

Hence, the eigenvalues of $\exp[R(q)(t-t_0)]$ are given by $\exp[\lambda(q)(t-t_0)]$, the eigenvectors remain unchanged, and:

$$\vec{p}(q,t) = D(q) \exp[\Lambda(q)(t-t_0)] D(q)^{-1} \vec{p}(q,t_0) \quad (29)$$

provided the decomposition (27) actually exists, i.e., N_{prim} different eigenvectors of $R(q)$ can be found. Indeed, this is always the case, as is shown next.

(g) Special eigenvectors; symmetrization of the matrices

Apart from being real, the matrix $R(q=0)$ enjoys the distinction of being singular, i.e., one eigenvalue vanishes. This zero eigenvalue is enforced by the conservation of probability (the probability to find the system in some configuration, after all, is unity at any time), and the corresponding eigenvectors are connected to the equilibrium occupation of the configurations (see the script dedicated to equilibrium properties of the diffusion problem).

Formally, we first show that a vector $\vec{n} = (\dots 1 1 1 \dots)^T$ composed of unit entries is a left eigenvector of $R(0)$.

This means $\vec{r}^T R(0) = \vec{0}^T$, or in other words, a vanishing column sum in $R(0)$. Indeed, summing over all primitives γ in (22), one finds:

$$\sum_{\gamma} R(\gamma, z; 0) = -R(z) + \sum_{\gamma} [R_D(\gamma, z) + R_G(\gamma, z)] = 0 \quad (30)$$

as follows from (16). The corresponding right eigenvector \vec{r}_{eq} fulfills $R(0) \cdot \vec{r}_{eq} = \vec{0}$ and, according to (25), remains unaffected by the temporal evolution of the system. It thus must represent the equilibrium distribution among the primitives z . (since R , in general, is not a symmetric matrix, see (15), left and right eigenvectors to the same eigenvalue are different)

We established that the equilibrium occupation of any configuration only depends on its number of contiguous atomic blocks m (see Section (c), equilibrium properties script) and is proportional to $(B/C)^m$. It is therefore invariant with respect to rotations of the pattern, and is a function of the associated primitive z only. In the momentum representation (18), the (unnormalized) equilibrium distribution then reads:

$$\begin{aligned} \langle (z|q) \rangle_{eq} &= \frac{1}{p} \left(\frac{B}{C}\right)^{m(z)} \sum_{v=0}^{p-1} e^{-2\pi i q v / p} \\ &= \left(\frac{B}{C}\right)^{m(z)} \delta(0, q_{mod}) \end{aligned} \quad (31)$$

Therefore, the elements of $\vec{r}_{eq}(q=0)$ are given by $\left(\frac{B}{C}\right)^{m(z)}$, apart from normalization.

Note that the left and right eigenvector become identical when $B=C$, but then, a glance at the symmetry relation (15) shows that $R_D(\gamma, z) = R_G(z, \gamma)$, and therefore, according to (22):

$$R(\gamma|z; q)_{B=C} = R(z|\gamma; q)^*_{B=C} \quad (32)$$

For $B=C$, the matrices $R(q)$ are hermitian, and left and right eigenvectors are conjugate complex. This property furthermore guarantees that all eigenvalues λ are real, and that there is a unitary matrix $U(q) = (U(q)^+)^{-1}$ so that in (27),

$$R(q)_{B=C} = U(q) \Lambda(q) U(q)^+ \quad (33)$$

The structure of the equilibrium eigenvectors suggests a simple strategy to symmetrize the matrices $R(q)$, which has the benefit of more stringent statements concerning the spectrum of $R(q)$, and allows diagonalization of these matrices using a sequence of numerically stable unitary transformations (see the description of the Householder tridiagonalization scheme and the iterative QR diagonalization algorithm). For example, if $R(q)$ is similar to a Hermitian matrix $\tilde{R}(q)$, then the formal diagonalization in (27) and the solution of the master equation in (28), (29) is always possible. Furthermore, the spectrum of $R(q)$ is then real. With (27), (33):

$$R(q) = S(q) \tilde{R}(q) S(q)^{-1} = [S(q) U(q)] \Lambda(q) [S(q) U(q)]^{-1} \quad (34)$$

where $S(q)$ is the symmetrizing matrix, and $D(q) = S(q) U(q)$ is the diagonalizing transformation matrix.

We start out with the principle of detailed balance, stating that the weighed jump rates between each pair of states must cancel in equilibrium:

$$R_D(\eta, \gamma) p_{eq}(\gamma) = R_G(\gamma, \eta) p_{eq}(\eta) \quad (35)$$

While (35) immediately yields a stationary solution to the master equation (17), one cannot conversely conclude that a stationary state \vec{p}_{eq} of the master equation does enforce detailed balance (35). E.g., (35) generally does not hold if the jump rates in the clockwise and counter-clockwise directions differ. So, we first verify (35) for the problem under consideration. Eq. (35) demands that

$$\frac{R_D(\eta, \gamma)}{R_G(\gamma, \eta)} = \frac{p_{eq}(\eta)}{p_{eq}(\gamma)} = \left(\frac{\gamma}{\eta}\right)^{\Delta m} \quad (36)$$

where $\Delta m = m(\eta) - m(\gamma)$. For $|\Delta m| \geq 2$, no jumps occur, and (35) trivially holds. Using the table on page 3, together with (15), it is easy to verify (36) for every single type of jump A, B, C, D.

In the next step, we rewrite (35) in the form:

$$\frac{1}{\sqrt{p_{eq}(y)}} R_D(y, z) \sqrt{p_{eq}(z)} = \frac{1}{\sqrt{p_{eq}(z)}} R_D(z, y) \sqrt{p_{eq}(y)} \quad (37)$$

and in the same vein, use (22) to define:

$$\tilde{R}(y, z; q) = \frac{1}{\sqrt{p_{eq}(y)}} R(y, z; q) \sqrt{p_{eq}(z)} \quad (38)$$

With (22) and (37), it follows at once that the modified rate coefficient matrix $\tilde{R}(q) = \tilde{R}(q)^*$ is hermitian:

$$\tilde{R}(y, z; q) = \tilde{R}(z, y; q)^* \quad (39)$$

and can therefore be diagonalized in the form (33). (Note that the off-diagonal elements of type B and C in $R(y, z; q)$ will be replaced by the geometric mean \sqrt{BC} in $\tilde{R}(y, z; q)$, while off-diagonal elements of type A and D, as well as all diagonal elements, remain unchanged.)

Defining the symmetrizing matrix $S = S(q)$ by:

$$S(y, z) = \sqrt{p_{eq}(y)} S_{yz}, \quad (40)$$

i.e. as a diagonal matrix, we find that

$$R(q) = S \tilde{R}(q) S^{-1} = S U(q) \Lambda(q) U(q)^+ S^{-1} \quad (41)$$

Hence, knowledge of the equilibrium eigenvector \vec{p}_{eq} of $R(0)$ permits to transform the problem into a simpler hermitian one.

(h) Example: One-particle diffusion

To illustrate the ideas presented so far, we start out with the simplest diffusion problem, viz., one particle on p sites arranged in a circle. There are p different ways to place this atom, but all arrangements are related by rotation,

so only a single primitive configuration \bar{z} exists. For vanishing pattern sum r , site 0 must be occupied, and the binary code of the primitive is $2^0 = 1$ (see page 8.)

As only an isolated atom is present, all jumps are of type A. The master equation (23) collapses into an ordinary differential equation:

$$\frac{d}{dt} \langle (\bar{z}|q) \rangle = R(\bar{z}, \bar{z}; q) \langle (\bar{z}|q) \rangle \quad (42)$$

where the rate coefficients are given by:

$$R_D(\bar{z}, \bar{z}) = R_G(\bar{z}, \bar{z}) = A, \quad (43)$$

from which $R(\bar{z}) = 2A$ follows (16), and subsequently:

$$\begin{aligned} R(\bar{z}, \bar{z}; q) &= -2A + e^{-2\pi i q/p} A + e^{2\pi i q/p} A \\ &= -4A \sin^2 \frac{\pi q}{p} \end{aligned} \quad (44)$$

(Note that the change of shift $\Delta v = [1/k]_{mod p} = 1_{mod p} = 1$ in (9), (23).) The elements in (44) are the eigenvalues of the problem, and the eigenvectors in momentum space, are unit vectors ($\mu = 0, 1, \dots, p-1$):

$$\lambda_\mu = -4A \frac{\sin^2 \frac{\pi \mu}{p}}{p}, \quad \langle (\bar{z}|q) \rangle_\mu = \delta_{q, \mu}. \quad (45)$$

The eigenstates of the diffusion problem in position space follow from (19) after normalization: in the case $\mu = 0$:

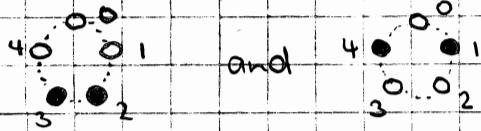
$$\langle [\bar{z}|v] \rangle_\mu = \frac{1}{p} e^{2\pi i \mu v / p} \quad (46)$$

and they are wave-like. In equilibrium, all configurations have equal probability $\langle [\bar{z}|v] \rangle_{eq} = 1/p$.

(i) Example: Two atoms on five sites

To demonstrate the working of the full apparatus on a problem that still allows solution in closed form, we calculate the

eigenvalues for the diffusion of two atoms ($k=2$) on five sites ($p=5$). There are $\binom{5}{2} = 10$ different arrangements of these atoms, but two sets of five configurations each are related through rotations and form equivalence classes, leaving essentially two different patterns. These are represented by the primitives:



Equivalent to the binary codes $01100 = 12$ and $10010 = 18$.
(Their pattern sums are $(2+3) \bmod 5 = (1+4) \bmod 5 = 0$, as required.)
In the pattern (12), both atoms form a block (block number $m=1$), whereas they are separate in pattern (18) ($m=2$). Their equilibrium occupation is thus given by:

$$f_{12}^{(\text{eq})} = 1/2, \quad f_{18}^{(\text{eq})} = (B/C)/2 \quad (47)$$

where the partition function Z is chosen so that the sum over all configurations yields unit probability: $Z = p \cdot (1 + B/C)$, or:

$$f_{12}^{(\text{eq})} = \frac{C}{p(B+C)}, \quad f_{18}^{(\text{eq})} = \frac{B}{p(B+C)} \quad (48)$$

Apart from rotations, the elementary jump events permitted for these patterns are

(i)			(J)	type B	$v=2$
(ii)			(P)	type B	$v=3$
(iii)			(J)	type A	$v=2$
(iv)			(C)	type C	$v=3$
(v)			(J)	type C	$v=2$
(vi)			(C)	type A	$v=3$

In the cases (i) and (ii), the resulting patterns belong to the (18) primitive class, starting from the primitive (12). Starting from the primitive (18), there are four possible jumps (in accordance with the counting scheme of Section (c), page 12). Jumps (iii) and (vi) produce a congruent pattern that is simply rotated with respect to the initial pattern and belongs to the same equivalence class,

while jumps (iv) and (v) yield members of the equivalence class belonging to the primitive (12). All clockwise jumps end up in patterns rotated by $v=3$ ticks from their primitive counterparts; indeed, with (5) we find $r = [v \cdot k]_{\text{mod } 5} = 6 \text{ mod } 5 = 1$, as required by a clockwise jump, and similarly $r = [z \cdot z]_{\text{mod } 5} = -1 \text{ mod } 5$ for all counterclockwise jumps. In accordance with the table on page 3, jumps that increase the block number are of the "B" type, jumps that decrease m are of type "C", and jumps within the same equivalence class are of type "A". (Events of the "D" kind require the presence of at least 3 atoms. There are $\binom{3}{1} = 3$ jumps in each direction (10), and they are distributed among A, B, and C [cf. (11), (12)].

The loss rates $R(z)$ for the two primitives (16) therefore are $R[(12)] = 2B$ and $R[(18)] = 2(A+C)$, respectively. The elements of the rate coefficient matrix (22) then read:

$$\begin{aligned} R[(12), (12); q] &= -2B \\ R[(12), (18); q] &= (e^{-6\pi i q/5} + e^{6\pi i q/5})C = 2C \cos\left(\frac{4\pi}{5}q\right) \\ R[(18), (12); q] &= (e^{-6\pi i q/5} + e^{6\pi i q/5})B = 2B \cos\left(\frac{4\pi}{5}q\right) \\ R[(18), (18); q] &= -2(A+C) + (e^{-6\pi i q/5} + e^{6\pi i q/5})A \\ &= -2C - 2A[1 - \cos\left(\frac{4\pi}{5}q\right)] = -2C - 4A \sin^2\left(\frac{2\pi}{5}q\right) \end{aligned} \quad (49)$$

(Note that $\cos \frac{6\pi q}{5} = \cos \frac{4\pi q}{5}$ for integer q .) Note that the rate matrix is real, but not symmetric, because $R[(12), (18); q]$ and $R[(18), (12); q]$ differ in the jump rate (B vs. C), see the table (15). To symmetrize it, we multiply with the matrix S (40) that is derived from the equilibrium occupations of the primitives (48). According to (38):

$$\begin{aligned} \tilde{R}(q) &= S^{-1} R(q) S \\ &= \begin{pmatrix} C^{-1/2} & 0 \\ 0 & B^{-1/2} \end{pmatrix} \begin{pmatrix} -2B & 2C \cos \frac{4\pi q}{5} \\ 2B \cos \frac{4\pi q}{5} & -2C - 4A \sin^2 \frac{2\pi q}{5} \end{pmatrix} \begin{pmatrix} C^{1/2} & 0 \\ 0 & B^{1/2} \end{pmatrix} \\ &= \begin{pmatrix} -2B & 2\sqrt{BC} \cos \frac{4\pi q}{5} \\ 2\sqrt{BC} \cos \frac{4\pi q}{5} & -2C - 4A \sin^2 \frac{2\pi q}{5} \end{pmatrix} \end{aligned} \quad (50)$$

The resulting matrix is indeed symmetric.

We now illustrate the working of the full diagonalization scheme for the case of zero momentum, $q=0$. Then, (50) simplifies to:

$$\tilde{R}(0) = \begin{pmatrix} -2B & 2\sqrt{BC} \\ 2\sqrt{BC} & -2C \end{pmatrix} \quad (51)$$

The characteristic polynomial here reads:

$$(\lambda + 2B)(\lambda + 2C) - 4BC = \lambda^2 + 2(B+C)\lambda = 0 \quad (52)$$

so that $\lambda_1(0) = 0$, and $\lambda_2(0) = -2(B+C)$. (λ , obviously represents the equilibrium eigenstate.) It is not difficult to find a pair of eigenvectors to (51) and normalize it; apart from the choice of sign they are unique and read:

$$\vec{u}_1 = \frac{1}{\sqrt{B+C}} \begin{pmatrix} \sqrt{C} \\ \sqrt{B} \end{pmatrix}, \quad \vec{u}_2 = \frac{1}{\sqrt{B+C}} \begin{pmatrix} -\sqrt{B} \\ \sqrt{C} \end{pmatrix} \quad (53)$$

As eigenvectors of a symmetric matrix they are orthogonal, $\vec{u}_1^T \cdot \vec{u}_2 = 0$. They form the columns of the unitary transformation matrix $U(0)$ in (41):

$$\tilde{R}(0) = \begin{pmatrix} \sqrt{\frac{C}{B+C}} & -\sqrt{\frac{B}{B+C}} \\ \sqrt{\frac{B}{B+C}} & \sqrt{\frac{C}{B+C}} \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & -2(B+C) \end{pmatrix} \begin{pmatrix} \sqrt{\frac{C}{B+C}} & \sqrt{\frac{B}{B+C}} \\ -\sqrt{\frac{B}{B+C}} & \sqrt{\frac{C}{B+C}} \end{pmatrix} \quad (54)$$

(Note that defining $\Theta = \arctg(\sqrt{B/C})$, we can restate $U(0)$ in the familiar form of a rotation matrix: $U(0) = \begin{pmatrix} \cos\Theta & -\sin\Theta \\ \sin\Theta & \cos\Theta \end{pmatrix}$.)

The diagonalization of the actual rate matrix $R(0)$ finally requires a similarity transform using S : $R(0) = D(0) \Lambda(0) D(0)^{-1}$ (27), where $D(0) = S U(0)$ (41), or:

$$R(0) = \frac{1}{P} \begin{pmatrix} \frac{C}{B+C} & -\frac{\sqrt{BC}}{B+C} \\ \frac{B}{B+C} & \frac{\sqrt{BC}}{B+C} \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & -2(B+C) \end{pmatrix} \cdot P \begin{pmatrix} 1 & 1 \\ -\sqrt{B/C} & \sqrt{C/B} \end{pmatrix} \quad (55)$$

Note that the first column of $D(0)$ contains the right equilibrium eigenvector $\vec{p}_{eq}(0)$ (48), and the first row of $D(0)^{-1}$ the left equilibrium eigenvector $\vec{p} \cdot \vec{m} = \vec{p}(11)^T$ [see section (8)]. The other

Column and row describe the decaying state with eigenvalue λ_2 . Note that the corresponding right eigenvector is orthogonal to \hat{n} ; its average number of atoms thus vanishes, guaranteeing conservation of probability in (29).

Next, we consider the rate coefficient matrices for non-vanishing momentum $q \neq 0$. Before we start the actual calculation, we remark that the rate matrix coefficients (49) are all real, a property that is linked to the invariance of the primitives (12) and (18) under mirror reflections [see separate script]. Together with the relation (24) this means that:

$$R(q=1) = R(q=4), \quad R(q=2) = R(q=3) \quad (56)$$

so that the eigenvalues and -vectors corresponding to these momenta are identical, and we may limit ourselves to the cases $q=1, 2$. Here, we are mainly interested in the eigenvalues of the problem. For $q=1$, the symmetrized matrix reads:

$$R(1) = \begin{pmatrix} -2B & -2\sqrt{BC} \cos \frac{\pi}{5} \\ -2\sqrt{BC} \cos \frac{\pi}{5} & -2C - 4A \sin^2 \frac{2\pi}{5} \end{pmatrix} \quad (57)$$

its characteristic polynomial is given by

$$\lambda^2 + 2(B+C+2A \sin^2 \frac{2\pi}{5})\lambda + 4B(C \sin^2 \frac{\pi}{5} + 2A \sin^2 \frac{2\pi}{5}) = 0 \quad (58)$$

and the eigenvalues $\lambda_{1/2}(q=1)$ are given by

$$\lambda_{1/2} = -(B+C+2A \sin^2 \frac{2\pi}{5}) \pm \sqrt{(B-C-2A \sin^2 \frac{2\pi}{5})^2 + 4BC \cos^2 \frac{\pi}{5}} \quad (59)$$

In the case $q=2$, we find with $\sin^2 \frac{4\pi}{5} = \sin^2 \frac{\pi}{5}$:

$$R(2) = \begin{pmatrix} -2B & -2\sqrt{BC} \cos \frac{2\pi}{5} \\ -2\sqrt{BC} \cos \frac{2\pi}{5} & -2C - 4A \sin^2 \frac{\pi}{5} \end{pmatrix} \quad (60)$$

and correspondingly,

$$\lambda^2 + 2(B+C+2A \sin^2 \frac{\pi}{5})\lambda + 4B(C \sin^2 \frac{2\pi}{5} + 2A \sin^2 \frac{\pi}{5}) = 0 \quad (61)$$

and for the eigenvalues $\lambda_{1/2}$ ($q=2$):

$$\lambda_{1/2} = - (B+C+2A \sin^2 \frac{\pi}{5}) \pm \sqrt{(B-C-2A \sin^2 \frac{\pi}{5})^2 + 4BC \cos^2 \frac{2\pi}{5}} \quad (62)$$

Note that they differ only in that the arguments of the trigonometric functions are exchanged.

It is instructive to examine some special cases in more detail:

(i) $B=0$ (sticky atoms)

If $B=0$, atoms attached to a block will never jump. In a sense, they are sticky — atoms in pairs and larger contiguous blocks are immobilized. Here, this means that the jumps of type (i) and (ii) on page 21 will never take place. In other words, all arrangements in the rotational equivalence class represented by primitive (12) are stationary states:



Correspondingly, the set of eigenvalues of the master equation (17) should contain $\lambda=0$ as a fivefold degenerate subspace. This is indeed true, as (52), (56), (59), (62) show. For $B=0$,

$$\begin{aligned}\lambda_1(0) &= 0, \quad \lambda_2(0) = -2C \\ \lambda_1(1) &= \lambda_1(4) = 0, \quad \lambda_2(1) = \lambda_2(4) = -2C - 4A \sin^2 \frac{2\pi}{5} \\ \lambda_1(2) &= \lambda_1(3) = 0, \quad \lambda_2(2) = \lambda_2(3) = -2C - 4A \sin^2 \frac{\pi}{5}.\end{aligned}\quad (63)$$

(ii) $C=0$ (site blocking)

If $C=0$, atoms are prohibited from attaching themselves to other atoms (or blocks of atoms). The sites next to an occupied site are unavailable, the jumps of type (iv) and (v) (see page 21) never take place. If the initial configuration is entirely contained in the equivalence class of primitive (18), then this property will hold at all times,

and the evolution takes place exclusively through jumps of type (iii) and (vi). Note that they can be interpreted as rotations of the entire pattern by $v = \pm 3$ units. Thus we expect that the dynamics then is equivalent to simple diffusion [Section (h)], except that the eigenvalues λ_μ (45) have to be corrected for the fact that the elementary event is a shift of the pattern of three sites, instead of one site in single-atom diffusion:

$$\lambda_\mu = -4A \sin^2 \frac{v\pi q}{p} = -4A \sin^2 \frac{3\pi q}{5} \quad (64)$$

The remaining five eigenvalues of the rate coefficient matrix (17) describe the decay of the primitive (12) (jumps of type (i) and (ii) on page 21), governed by the decay rate B .

Indeed, the eigenvalues according to (52), (59) and (62) are:

$$\begin{aligned} \lambda_1(0) &= 0, \quad \lambda_2(0) = -2B \\ \lambda_1(1) &= \lambda_1(4) = -4A \sin^2 \frac{2\pi}{5}, \quad \lambda_2(1) = \lambda_2(4) = -2B \\ \lambda_1(2) &= \lambda_1(3) = +4A \sin^2 \frac{\pi}{5}, \quad \lambda_2(2) = \lambda_2(3) = -2B \end{aligned} \quad (65)$$

Since $\sin^2 \frac{2\pi}{5} = \sin^2 \frac{3\pi}{5}$, and $\sin^2 \frac{\pi}{5} = \sin^2 \frac{6\pi}{5}$, this result coincides with (64).

(iii) $A=B=C$ (simple diffusion)

If $A=B=C$, all jumps take place with a single frequency, independent of the occupation of the neighbouring sites. In this case, it is instructive to perform some non-trivial mathematical transformations first. We start out with a geometrical series similar to (18), (19):

$$e^{-4\pi i/5} + e^{-2\pi i/5} + 1 + e^{2\pi i/5} + e^{4\pi i/5} = 0 \quad (66)$$

One may rewrite this into trigonometrical identities:

$$1 + \cos \frac{2\pi}{5} + \cos \frac{4\pi}{5} = \frac{1}{2} \quad (67)$$

$$1 - \cos \frac{\pi}{5} + \cos \frac{2\pi}{5} = \frac{1}{2} \quad (68)$$

(since $\cos \frac{\pi}{5} = -\cos \frac{4\pi}{5}$), and furthermore with $\cos 2x = 2\cos^2 x - 1$, (27)

$$\cos^2 \frac{\pi}{5} - \frac{1}{2} \cos \frac{\pi}{5} - \frac{1}{4} = 0 \quad (69)$$

$$\cos^2 \frac{2\pi}{5} + \frac{1}{2} \cos \frac{2\pi}{5} - \frac{1}{4} = 0 \quad (70)$$

From these, it is easy to establish algebraic expressions for the trigonometric functions:

$$\cos \frac{\pi}{5} = \frac{1}{4}(\sqrt{5} + 1), \quad \cos \frac{2\pi}{5} = \frac{1}{4}(\sqrt{5} - 1) \quad (71)$$

$$\sin^2 \frac{\pi}{5} = \frac{\sqrt{5}}{8}(\sqrt{5} - 1), \quad \sin^2 \frac{2\pi}{5} = \frac{\sqrt{5}}{8}(\sqrt{5} + 1) \quad (72)$$

From that, the identities:

$$(\sin^2 \frac{2\pi}{5} + \cos \frac{2\pi}{5})^2 = \sin^4 \frac{2\pi}{5} + \cos^2 \frac{\pi}{5} \quad (73)$$

$$(\sin^2 \frac{\pi}{5} - \cos \frac{\pi}{5})^2 = \sin^4 \frac{\pi}{5} + \cos^2 \frac{2\pi}{5} \quad (74)$$

are easily verified.

Equations (73) and (74) are helpful in interpreting the eigenvalues occurring in the simple diffusion of two atoms on five sites. While in the zero-momentum subspace ($q=0$),

$$\lambda_1(0) = 0, \quad \lambda_2(0) = -4A \quad (75)$$

holds (52), we obtain with (59) and (73) for $q=1$:

$$\begin{aligned} \lambda_{1,2}(1) &= -2A(1 + \sin^2 \frac{2\pi}{5}) \pm 2A \sqrt{\sin^4 \frac{2\pi}{5} + \cos^2 \frac{\pi}{5}} \\ &= -2A \left[1 + \sin^2 \frac{2\pi}{5} \mp (\sin^2 \frac{2\pi}{5} + \cos^2 \frac{2\pi}{5}) \right] \end{aligned} \quad (76)$$

or, with $1 - \cos x = 2 \sin^2 \frac{x}{2}$, $1 + \cos x = 2 \cos^2 \frac{x}{2}$,

$$\lambda_1(1) = -4A \sin^2 \frac{\pi}{5} = -\frac{\sqrt{5}}{2}(\sqrt{5} - 1)A \quad (77)$$

$$\lambda_2(1) = -4A(\sin^2 \frac{2\pi}{5} + \cos^2 \frac{\pi}{5}) = -(4 + \sqrt{5})A \quad (78)$$

In a similar fashion, (61) and (74) yield in the case $q=2$:

(28)

$$\begin{aligned}\lambda_{12}(2) &= -2A\left(1+\sin^2\frac{\pi}{5}\right) \pm 2A\sqrt{\sin^4\frac{\pi}{5} + \cos^2\frac{2\pi}{5}} \\ &= -2A\left[1+\sin^2\frac{\pi}{5} \mp (\sin^2\frac{\pi}{5} - \cos\frac{\pi}{5})\right]\end{aligned}\quad (79)$$

Since $\cos^2\frac{\pi}{10} = \sin^2(\frac{\pi}{2} - \frac{\pi}{10}) = \sin^2\frac{2\pi}{5}$, we find:

$$\lambda_1(2) = -4A\sin^2\frac{2\pi}{5} = -\frac{\sqrt{5}}{2}(\sqrt{5}+1)A \quad (80)$$

$$\lambda_2(2) = -4A\left(\sin^2\frac{\pi}{5} + \cos^2\frac{2\pi}{5}\right) = -(4-\sqrt{5})A \quad (81)$$

Remarkably, (75), (77), and (80) show that each of the momentum subspaces in the $p=5, k=2$ problem contains the corresponding eigenvalue of the simple diffusion problem for a single atom [Section (h)] as a special member (45). As we shall show later (separate script), this invariably happens whenever the jump rates become equal ($A=B=C=D$).

(j) The evolution of occupation averages

In this section, we schematically gather the steps required to calculate the evolution of the average for a given arrangement of atoms and unoccupied sites, in the following called a comparison pattern. Such a pattern is composed of sites that have to be occupied (•), sites that are enforced to be empty (○), and sites whose occupation state remains unspecified (x). We adopt the convention that sites not explicitly defined in the pattern are supposed to be unspecified, i.e., of the "x" type.

It is useful to introduce two patterns derived from the comparison pattern, the "atom pattern" and the "hole pattern." The former is a pattern that has atoms at the sites prescribed by the comparison pattern, and holes (empty sites) elsewhere; the latter sports holes at all empty sites specified by the comparison pattern, and atoms on all other sites. Clearly, the atom pattern and hole pattern uniquely specify the comparison pattern, but unlike the comparison pattern itself allow encoding in the binary scheme introduced in Section (b), page 8.

As an example, consider the $p=11$ comparison pattern:

$\begin{matrix} \times & \times & \bullet & \circ & \circ & \bullet & \times & \times & \circ & \bullet & \times \\ 10 & 9 & 8 & 7 & 6 & 5 & 4 & 3 & 2 & 1 & 0 \end{matrix}$

or, in short form, $(\bullet\circ\circ\bullet\circ\circ\bullet\circ\bullet)$. (The index indicates the starting site of the sequence.) The assigned atom and hole patterns are, respectively:

$\begin{matrix} \circ & \circ & \bullet & \circ & \circ & \bullet & \circ & \circ & \circ & \bullet & \circ \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \end{matrix}$ (binary code $00100100010 = 290$)

$\begin{matrix} \bullet & \bullet & \bullet & \circ & \circ & \bullet & \bullet & \circ & \circ & \bullet & \bullet \\ 1 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 1 & 1 & 0 \end{matrix}$ (binary code $11100111011 = 827$)

A given atomic arrangement matches the comparison pattern if atoms are present at the atomic entries in the atom pattern, and the sites specified as holes in the hole pattern are all empty. Using the binary codes, this can be easily verified by bitwise logical operations. If (n) is the binary code of the arrangement, it will match the pattern if and only if the two conditions:

$$\begin{aligned} (n) \text{ AND } (\text{atom pattern code}) &= (\text{atom pattern code}) \\ (n) \text{ OR } (\text{hole pattern code}) &= (\text{hole pattern code}) \end{aligned}$$

are fulfilled simultaneously.

In this way, a table for all $\binom{P}{k}$ configurations [primitive z | shift v] (4) can be established that indicates whether the configuration matches the comparison pattern.

The general algorithm towards the evaluation of averages then is laid out as follows:

- (i) Establish an ordered list of primitive patterns z_f (page 7)
- (ii) Determine the block number $m(z)$ of each primitive z ; use it to create the equilibrium occupation vector \vec{x}_{eq} [see Section (g); also eq. (22) in the script on equilibrium probabilities]
- (iii) Examine all possible clockwise and counterclockwise jumps $R_C(z, z_f)$, $R_G(z, z_f)$ (14) for all primitives z_f , establish the loss term $R(z)$ (16), and store them in an array.

- (iv) Set up the real rate matrix for zero momentum ($q=0$) $R(0)$ (22), symmetrize it using the equilibrium eigenvector \vec{f}_{eq} (38), and use numerical techniques (Householder tridiagonalization, QR algorithm) to establish its eigenvalues $\Lambda(0)$ and the orthogonal transformation matrix $U(0)$:

$$\tilde{R}(0) = U(0) \Lambda(0) U(0)^T \quad (41).$$
- (v) Set up the complex rate matrices $R(q)$ for $q=1, 2, \dots, \frac{p-1}{2}$ (22), bring them in Hermitian form $\tilde{R}(q)$ using the equilibrium occupation factor (38), diagonalize them (Householder tridiagonalization, QR algorithm) to establish their eigenvalues $\Lambda(q)$ and the unitary transformation matrices $U(q)$:

$$\tilde{R}(q) = U(q) \Lambda(q) U(q)^+ \quad (41).$$
- (vi) If desired, (anti-)symmetrize the eigenvectors in the orthogonal matrix $U(0)$ [see separate script on symmetry properties]
- (vii) Use symmetry properties of primitives to store the unitary matrices $U(q)$, $q=1, 2, \dots, \frac{p-1}{2}$, in a compressed format [see separate script]
- (viii) Create a lookup table that contains matching information for each average to be calculated, and each primitive β and shift ν (see above)
- (ix) Translate the initial configuration $\langle [\beta | \nu] \rangle(t_0)$ into momentum-space averages $\langle (\beta | q) \rangle(t_0)$ (18), to form the $(p+1)/2$ initial vectors $\vec{f}(q, t_0)$.
- (x) Multiply these vectors with the diagonal symmetrizing matrix S^{-1} (41), and subsequently with the respective unitary transformation matrices $U^+(q)$ (41).
- (xi) For each timestep t , multiply the vectors with the diagonal matrix $\exp[\Lambda(q)(t-t_0)]$.
Note: If only the deviation from equilibrium is of interest, delete the diagonal entry in $\exp[\Lambda(0)(t-t_0)]$ corresponding to the equilibrium eigenvector $\vec{f}_{eq}(0)$.
- (xii) Multiply the vectors with the matrices $U(q)$ and the symmetrizing matrix S (41), to obtain the vectors $\vec{f}(q, t)$.
- (xiii) Project the occupations $\vec{f}(q, t)$ back onto configuration space $\langle [\beta | \nu] \rangle(t)$ (19).
- (xiv) For each average to be calculated, sum over the occupation probabilities $\langle [\beta | \nu] \rangle(t)$ of all matching arrangements.