Example: Evolution of one-site averages ($k=5$, $p=19$)

As an example of the algorithm, we considered the temporal evolution of a system of 5 atoms on a circular arrangement of 19 sites. Initially, the atoms form a compact block on the sites 17, 18, 0, 1, 2, and then are allowed to spread out. Here, we plotted the average occupation of the sites 0–9. (The occupation of the remaining sites follows by symmetry considerations.)

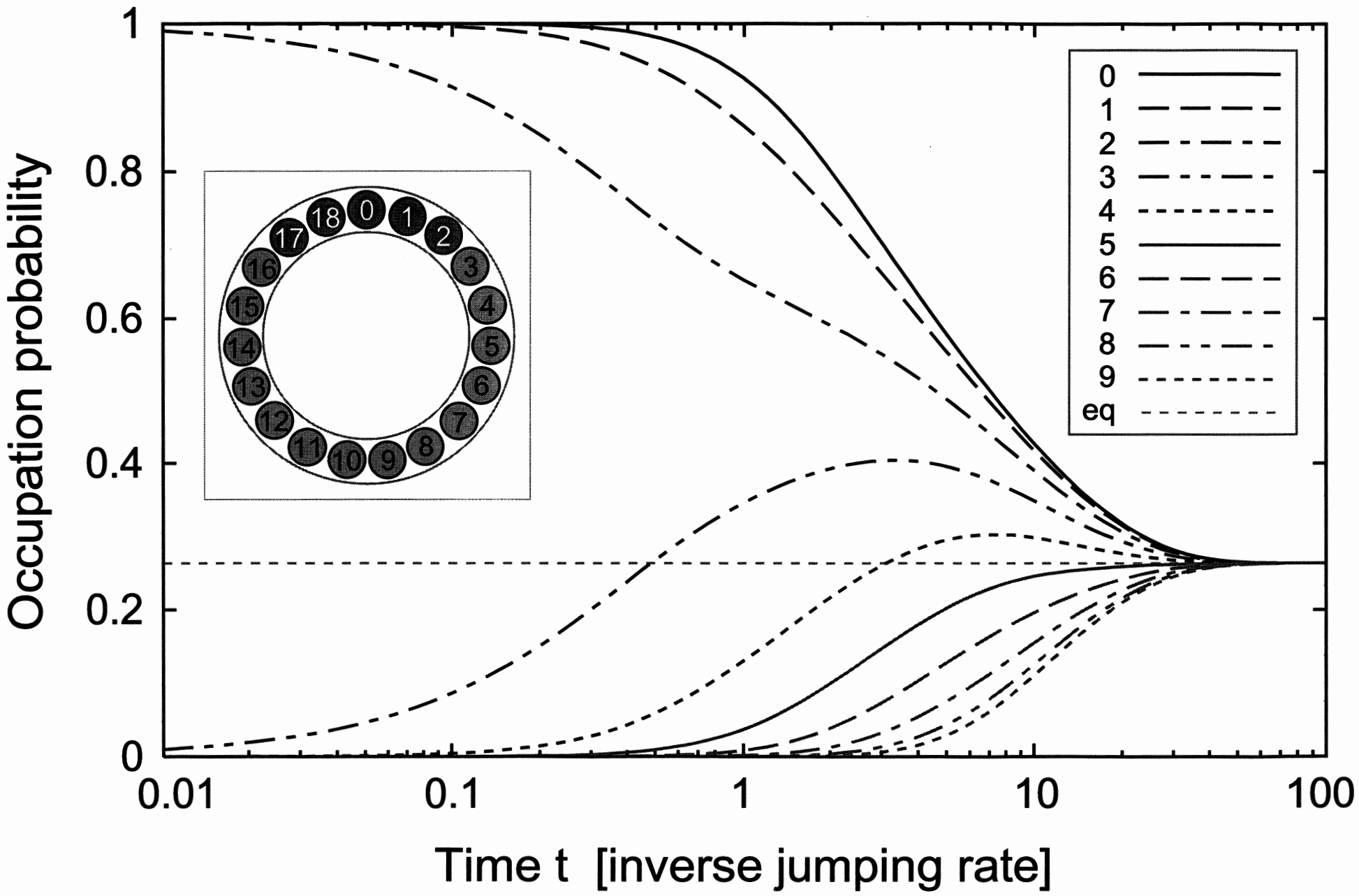
To illustrate the complexity and performance of the algorithm, we note that the problem has 11.628 distinct configurations in 612 primitives; the memory requirements for the transformation matrix (that dominate memory consumption) are $10 \cdot 612^2 = 3.745.440$ double-accuracy floats, stored in ~28.6 MByte. Complete diagonalization of the matrix takes about 36 minutes on a 400 MHz Pentium II PC.

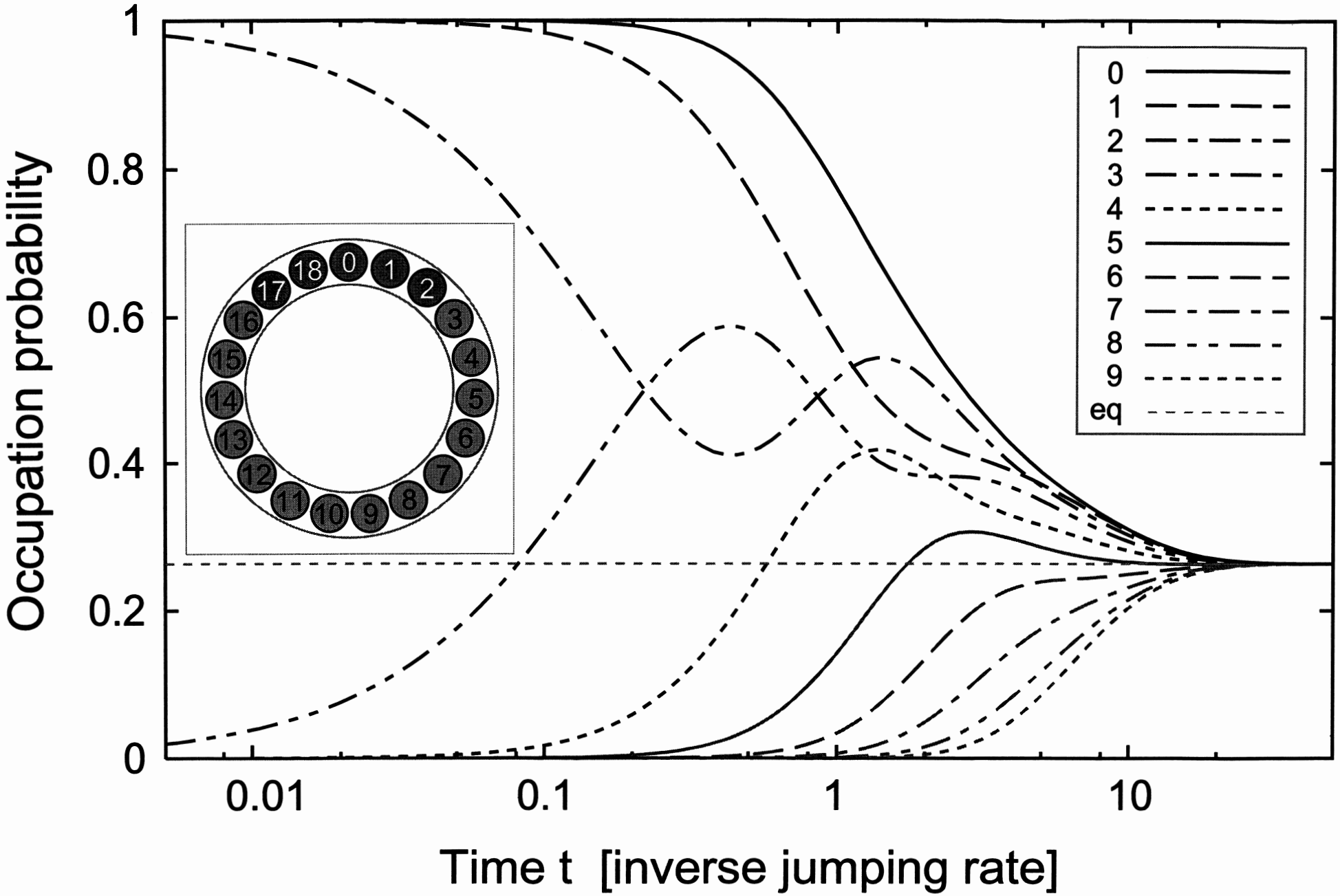
The plots show the results for different values of the jump rates B and C. (The rates A and D were held constant at unit value.)

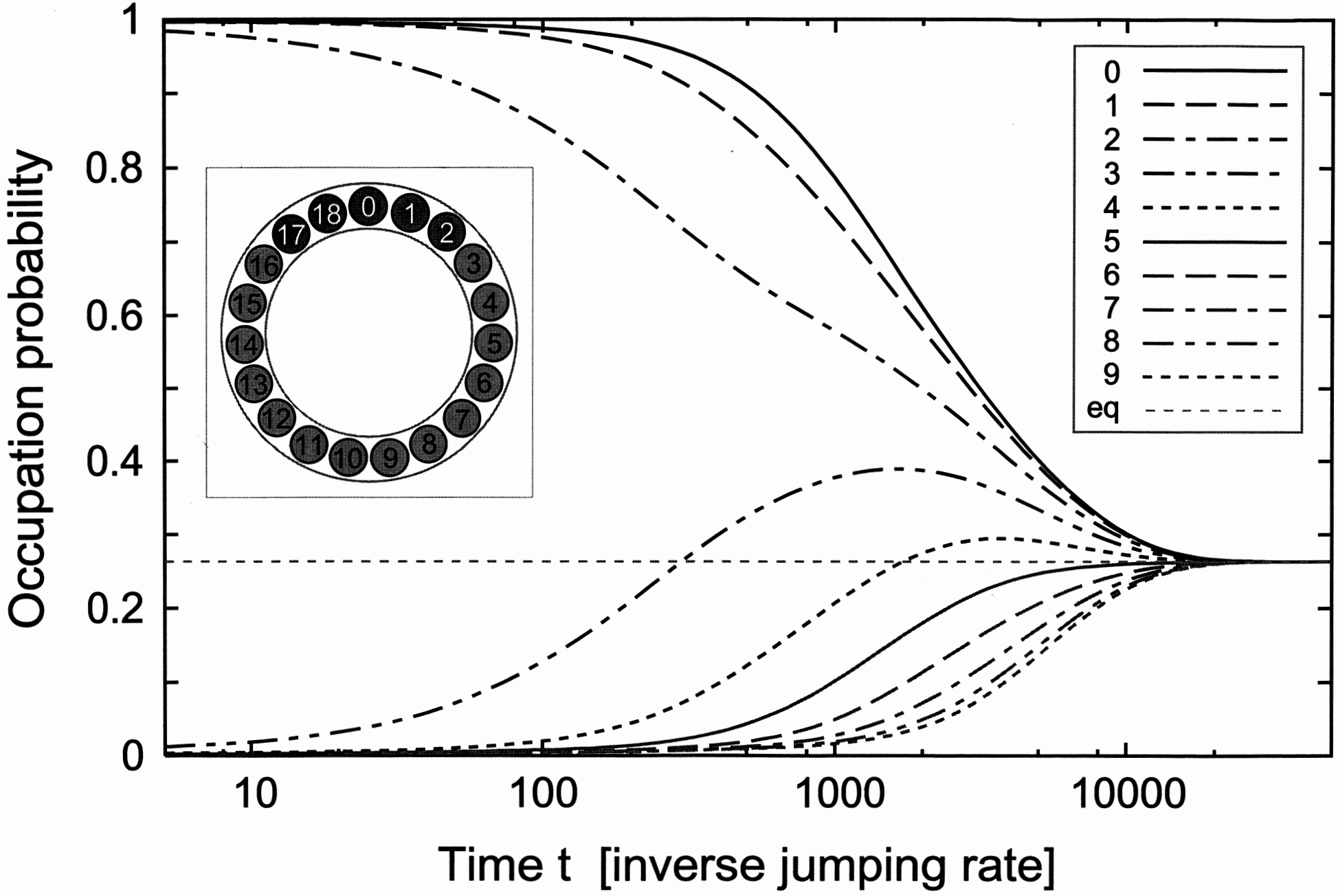
For $A=B=C=D=1$, simple diffusion takes place. The single site occupancies then follow the same evolution as a single atom [see script on simple diffusion, Section (a)], and the long-time behaviour is controlled by the smallest eigenvalue $\lambda_1 = -4A\sin^2(\pi/19) \approx 0.1084$.

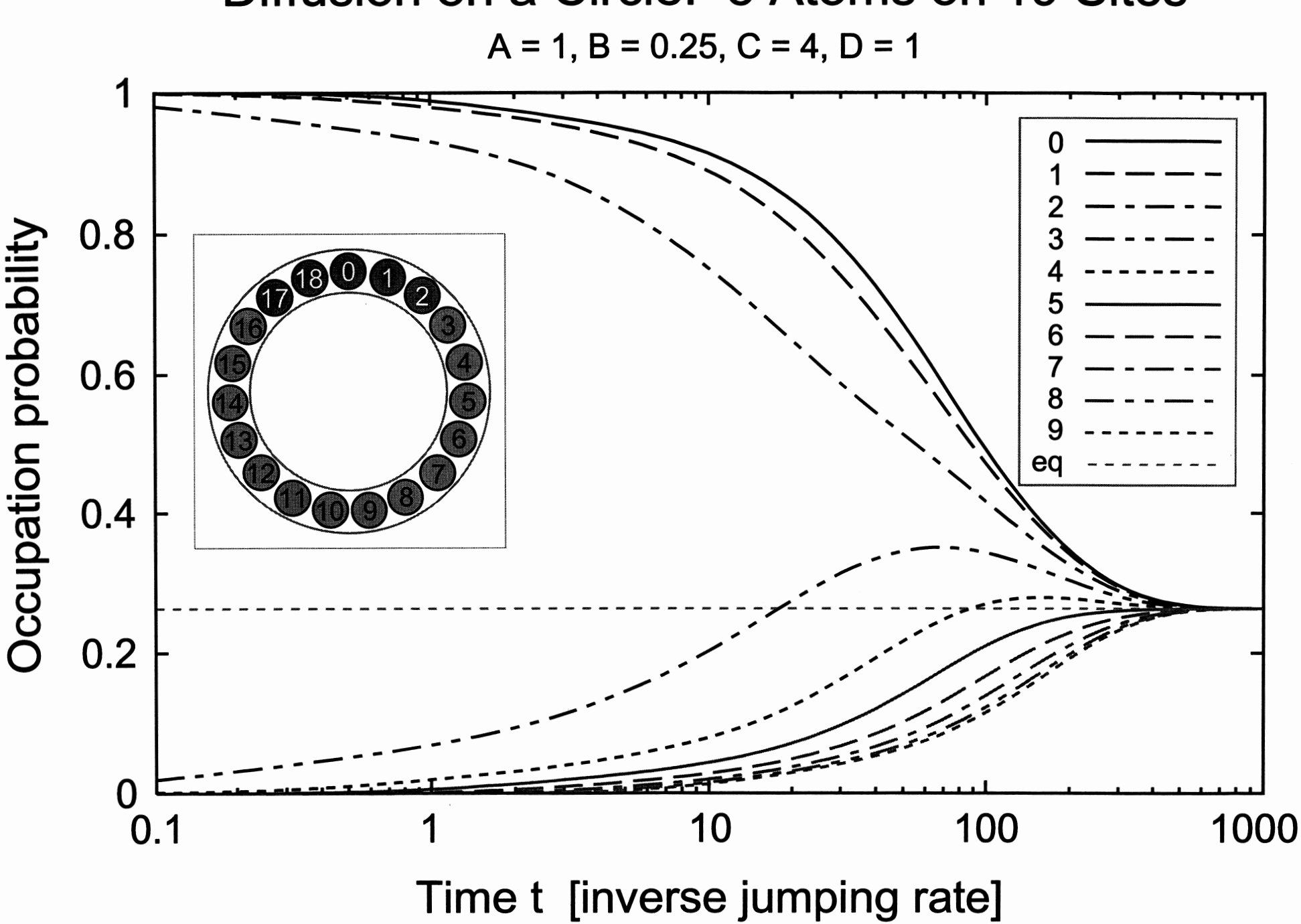
With decreasing ratio B/C, "evaporation" of atoms from contiguous blocks of atoms is suppressed, leading to increased equilibration times. Interestingly, as $B/C \to 0$, the shape of the occupancy curves becomes more and more similar to the simple diffusion case $B=C$ (albeit at different timescales). This feature may be explained by recalling that the system spends most of its time in a "condensed" state where the atoms occupy neighbouring sites. The evolution of the system then may be interpreted as the diffusion of this "quasiparticle." But for one-site averages, the diffusion of a single atom, and simple diffusion of a number of atoms, are analogous processes governed by the same master equation.

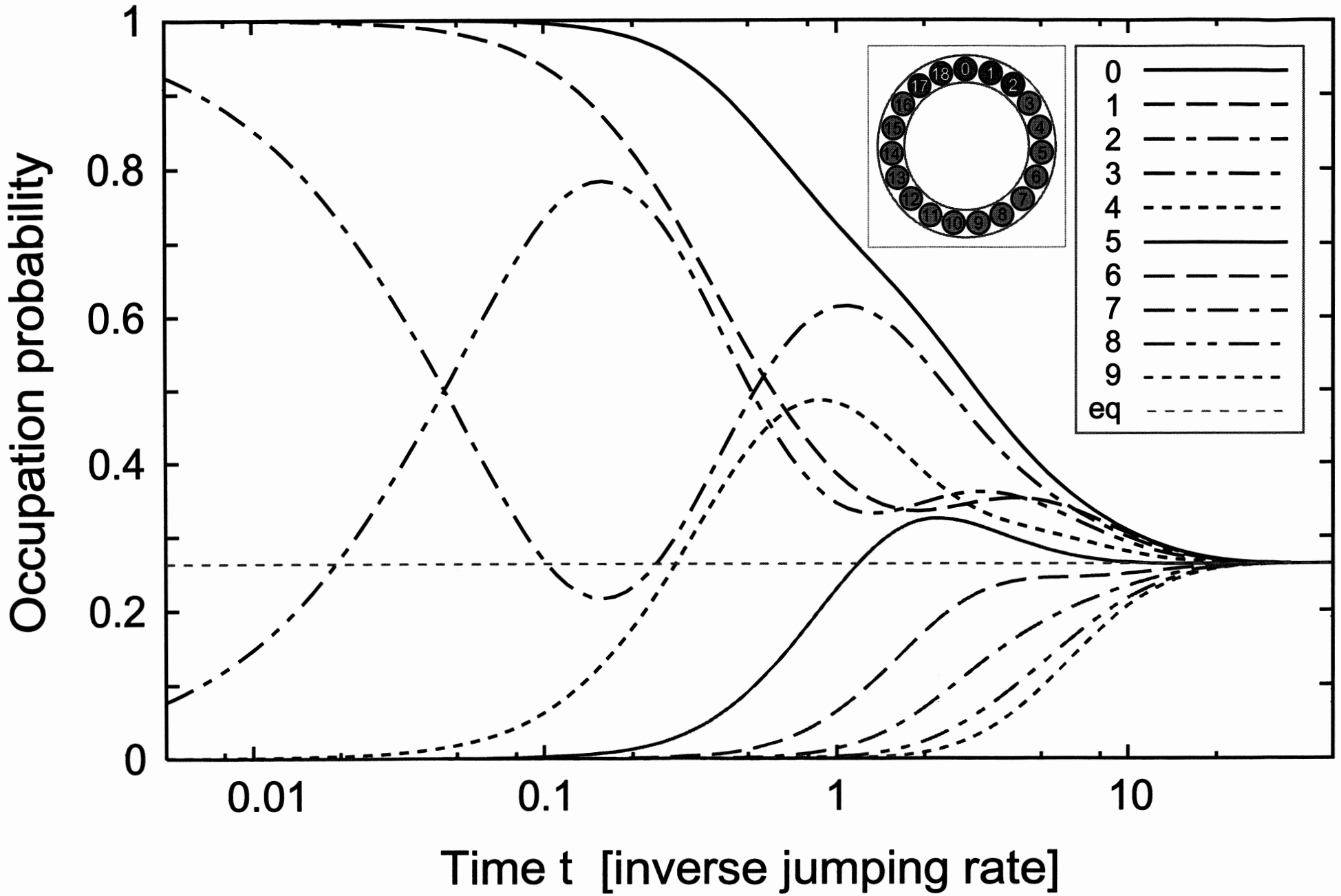
If the ratio B/C becomes greater than one, the atoms effectively repel each other. The outermost atoms then are pushed along the circle, leading to accelerated equilibration, while the "inner" atoms of the original pattern redistribute themselves. Interestingly, the interplay between repulsion and expansion creates transient oscillations in the site occupation probabilities that are absent in simple diffusion, and are rather unexpected.


Diffusion on a Circle: 5 Atoms on 19 Sites
A = 1, B = 1, C = 1, D = 1
Occupation probability
1
0.8
0.6
0.4
0.2
0
0.01
0.1
1
10
100
Time t [inverse jumping rate]
0
1
2
3
4
5
6
7
8
9
eq
18
17
16
15
14
13
12
11
10


Diffusion on a Circle: 5 Atoms on 19 Sites
A = 1, B = 4, C = 0.25, D = 1
Occupation probability
Time t [inverse jumping rate]
0
0.2
0.4
0.6
0.8
1
0.01
0.1
1
10
0
1
2
3
4
5
6
7
8
9
eq
18
17
16
15
14
13
12
11
10


Diffusion on a Circle: 5 Atoms on 19 Sites
A = 1, B = 1/16, C = 16, D = 1
Occupation probability
1
0.8
0.6
0.4
0.2
0
10
100
1000
10000
Time t [inverse jumping rate]
0
1
2
3
4
5
6
7
8
9
eq
18
0
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17


Diffusion on a Circle: 5 Atoms on 19 Sites
A = 1, B = 0.25, C = 4, D = 1
Occupation probability
Time t [inverse jumping rate]
0
0.2
0.4
0.6
0.8
1
0.1
1
10
100
1000
0
1
2
3
4
5
6
7
8
9
eq
18
17
16
15
14
13
12
11
10


Diffusion on a Circle: 5 Atoms on 19 Sites
A = 1, B = 16, C = 1/16, D = 1
Occupation probability
1
0.8
0.6
0.4
0.2
0
0.01
0.1
1
10
Time t [inverse jumping rate]
0
1
2
3
4
5
6
7
8
9
eq