Random Sequential Adsorption

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The explicit derivation of random sequential adsorption in one-dimension is presented.

Consider a random sequential adsorption process of deposition of particles of length k lattice sites on an infinite lattice. One way to derive the time evolution of the coverage is to consider the quantity $P(m,k,t)$ which is the probability that for any randomly chosen segment of m contiguous sites, that this segment is completely within a gap of length m or greater. In other words, if I randomly chose m adjacent, contiguous sites at time t, $P(m,k,t)$ is the probability that all of the sites are sites not covered by the length k particles. For an infinite lattice $L \to \infty$, and $m \ll L$, this is equivalent to scanning a window of m contiguous sites a large distance $\gg m$, one site at a time, across the lattice and counting the number of times all m sites are completely uncovered. This number, divided by the number of sites scanned asymptotically approaches $P(m,k,t)$ if the number of sites scanned $\gg m$.

Now consider how the quantity $P(m,k,t)$ evolves in time as particles are being deposited with unit rate. The deposition a particle on the lattice occurs only if there are at least k contiguous sites for the particle to insert. Otherwise, deposition or site covering occurs.

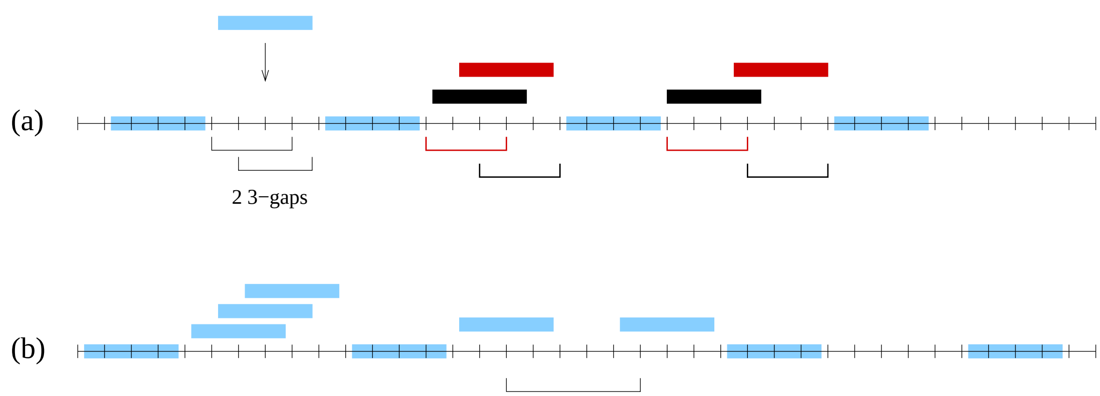

FIG. 1: (a) Gap dynamics for $m = 3 < k = 4$. (b) Gap dynamics for $m = 5 > k = 4$.

First consider the case $m < k$. As a concrete example, assume $m = 3$ and $k = 4$. The effects of the deposition of $k = 4$ particles on gaps of length $m = 3$ or more, are shown in Fig 1(a). Deposition of a long particle can cover segments completely within the length k. In this case, the deposition of a single particle of length k destroys $(k-m+1)$ contiguous gaps of length m or greater from the lattice. Deposition of a particle also destroys a gap of length m or greater if such a gap overlaps the region on which the k-mer adsorbed. This can happen in two ways. The overlapping can occur at either ends of the deposited particle. These destruction events are independent of the ones described by gaps that fall entirely within the k sites covered by the deposited particle only if gaps with length of at least $(k-m+1)$ are considered. Thus, the evolution equation for $P(m,k,t)$ is

$$\dot{P}(m,k,t) = -(k-m+1)P(k,k,t) - 2\sum_{j=1}^{m-1} P(k+j,k,t), \quad m < k. \tag{1}$$

Now consider the case where $m \geq k$, as shown in Fig. 1(b). Consider the case $m = 6$. by depositing a particle completely within a gap of $m = 6$ or greater, the gap can be destroyed in $(m - k + 1)$ ways. Particles that deposit overlapping parts of the ends of a length m subgap can also decrease the number of length m subgaps, as shown in Fig. 1(b). The subgap of length $m = 5$ is destroyed by particles of length $k = 4$ that deposit in such a way as to cover a few end sites of the $m = 5$ subgap. Thus, for $m \geq k$, we find

$$\dot{P}(m,k,t) = -(m-k+1)P(m,k,t) - 2\sum_{j=1}^{k-1} P(m+j,k,t), \quad m \geq k. \tag{2}$$

The initial condition is obviously $P(m,k,t=0) = 1$. These equations can be solved by assuming the form

$$P(m,k,t) = e^{-(m-k+1)t}F(k,t). \tag{3}$$

Upon substitution, Eq. 2 gives

$$F(k,t) = \exp\left[-2\sum_{j=1}^{k-1}\left(\frac{1-e^{-jt}}{j}\right)\right]. \tag{4}$$

Similarly, for $m < k$, we find

$$P(m,k,t) = 1 - \int_0^t \mathrm{d}u \left[(k-m+1) + 2\sum_{j=1}^{m-1} e^{-ju}\right] e^{-u}F(k,u). \tag{5}$$

The coverage is defined as

$$\theta(k,t) = 1 - P(1,k,t). \tag{6}$$

Consider the deposition of dimers ($k = 2$):

$$P(1,2,t) = 1 - 2e^{-2}\int_0^t \mathrm{d}u e^{-u}\exp\left[2e^{-u}\right] = \exp\left[-2+2e^{-t}\right] \tag{7}$$

In the $t \to \infty$ limit, we find $P(1,2,\infty) = e^{-2}$ and

$$\theta(k=2,\infty) = 1 - e^{-2} = 0.864665... \tag{8}$$

What is the coverage in the continuous case? Take the $k \to \infty$ limit.