I. MODEL

A. Overview

At every iteration, steps:

1. The set of allowed sites are calculated for all kind of processes.
2. The transition matrices are calculated for all available sites and channels for allowed processes.
3. The transition amplitudes are computed that are used with corresponding energetic penalties to find the transition rates.
4. A transition is selected stochastically and the quantum state and the sets of D,ϕ, and $\mathcal{A}$ is changed accordingly.

Electron hops to the right and left are treated separately.

II. TRANSITION MATRICES

Spin sectors:
For N active sites ($\mathcal{A}$) and m excitations, the basis states are made of sets of basis with $k \in [0, min(m, N)]$ sites in $\uparrow$ state and indexed in lexicographic order. The transition matrix maps are calculated for each of such set and combined to make full matrix.

A. D hops right/left

An electron hops from a D site to an active site. The active site becomes D and vice versa, the index of the initially active site is assigned to the new active site.
Transition matrix elements:
The basis states that have final site $\uparrow$ would allow an electron hopping to its HOMO level and create a D. This hop leaves the initially D site in $\uparrow$ (channel 1) or $\downarrow$ (channel 3). Similarly, the basis states that have final site $\downarrow$ would allow an electron hopping to its LUMO level and create a D. This hop leaves the initially D site in $\downarrow$ (channel 2) or $\uparrow$ (channel 4).

B. ϕ hops right/left

An electron hops from an active site to a ϕ. The active site becomes ϕ and vice versa, the index of the initially active site is assigned to the new active site.
Transition matrix elements:
The basis states that have the active site $\uparrow$ would allow the electron hopping from it and change it to ϕ. This hop makes the initially ϕ site in $\uparrow$ (channel 2) or $\downarrow$ (channel 3). Similarly, The basis states that have the active site $\downarrow$ would allow the electron hopping from it and change it to ϕ. This hop makes the initially ϕ site $\downarrow$ (channel 1) or $\uparrow$ (channel 4).

C. (D,ϕ) creation:

For two adjacent active sites, we can have four configurations: $(\uparrow,\downarrow)$, $(\downarrow,\uparrow)$,$(\uparrow,\uparrow)$,$(\downarrow,\downarrow)$ with left and right sites in (left,right) order. These will make (D,ϕ) pair with D on the left with the hopping of an electron from right to left via H-H, L-L, L-H, and H-L channels. Similarly, a (D,ϕ) pair with D on the right is created from these configurations with the hopping of an electron from left to right via L-L, H-H, L-H, and H-L channels, respectively.
Transition matrix elements:
The map between basis states of initial and final Hilbert spaces $\mathcal{H}_{N,m}$ and $\mathcal{H}_{N-2,m'}$, where $m' = m, m, m-1, m-2$ for H-H, L-L, L-H, H-L channels, can be calculated by starting from the final basis states in $\mathcal{H}_{N-2,m'}$ and inserting

the two active sites at their position in desired configuration ((↑,↓), etc.) to make the initial basis state. Let's call the combination of ↑ sites in the latter *set* and its lexicographic index in this m-th spin sector x, then

$$x = c_k^N - \sum_{p=0}^{k-1} c_{k-p}^{N-set(p)}. \tag{1}$$

D. (D,ϕ) annihilation:

This is just the reverse of (D,ϕ) creation described above where two active sites are created from a pair of D and ϕ. The freshly added active sites are given the indices $N+1, N+2$ and the map for the transition matrix is computed just like (D,ϕ) creation case. Since the electron hopping does not occur on active sites in this case, a single (D,ϕ) pair can be used to calculate the transition matrix and amplitudes.

E. D/ϕ creation at contacts:

If the site adjacent to a contact is active, it can gain or loose an electron via hopping from/to the contact to become a D or ϕ. The basis states with this site ↓ can get an electron from the contact (hopping parameter $J_{l,R/L}$; $RandL$ for right and left contacts) and become D or it can loose the electron to the contact (hopping parameter $J_{h,R/L}$) and become ϕ resulting in one less active site $N \to N-1$ and m unchanged. That is, the final state is in $\mathcal{H}_{N-1,m}$. The transition matrix map is obtained simply by starting with the basis in $\mathcal{H}_{N-1,m}$, inserting an ↓ in correct position to make the state in $\mathcal{H}_{N,m}$, and calculating its lexicographic index. Similarly, the basis states with this active site ↑ are linked via $J_{h,R/L}$ and $J_{l,R/L}$ to the basis in $\mathcal{H}_{N-1,m}$ for creation of D and ϕ respectively. The transition matrix map is calculated the same way.

F. D/ϕ annihilation at contacts:

These are just the reverse of D/ϕ creation at the contacts. A D or ϕ site adjacent to a contact becomes active on loosing or gaining an electron to/from it. Starting with D, the basis states in $\mathcal{H}_{N,m}$ are linked via $J_{l,R/L}$ ($J_{h,R/L}$) to the basis in $\mathcal{H}_{N+1,m'}$ with $m' = m\,(m+1)$ with this site being ↓ (↑). For a ϕ, the same transition map results with $J_{l,R/L} \leftrightarrow J_{h,R/L}$.