SUPPLEMENTARY MATERIAL for “Evolutionary dynamics of the prisoner’s dilemma with expellers”

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Contents

1 Extended pair approximation method for strategy updating dynamics 2
  1.1 Updating the strategy of a defector .................................................. 2
  1.2 Updating the strategy of a cooperator ............................................ 6
  1.3 Updating the strategy of an expeller ............................................. 10
  1.4 Master equations describing strategy updating dynamics ................. 14
1 Extended pair approximation method for strategy updating dynamics

In this supplementary material, we would like to present an extended pair approximation method for exploring strategy updating dynamics on regular graphs when \( w \to 0 \). When \( w \to 0 \), the pairwise interaction dynamics proceeds much faster than the strategy updating dynamics. Hence, the whole system enters into the equilibrium state that is only governed by pairwise interaction dynamics before it goes to the strategy updating phase. This means that the stationary regime of pairwise interaction dynamics determines the local configurations and the average payoffs of individuals (see APPENDIX B in main text). Let \( p_E, p_C, p_D \) and \( p_\phi \) denote the density of expellers, cooperators, defectors and vacant sites in a population, respectively. Let \( p_{EE}, p_{EC}, p_{CE}, p_{CC}, p_{ED}, p_{DE}, p_{DD}, p_{E\phi}, p_{\phi E}, p_{\phi C}, p_{CD}, p_{DC}, p_{C\phi}, p_{D\phi} \) and \( p_{\phi D} \) represent the stationary density of EE, EC, CE, CC, ED, DE, DD, E\phi, \phi E, \phi C, CD, DC, C\phi, D\phi and \phi D pairs resulted from pairwise interaction dynamics, respectively. Then \( q_{XY} = p_{XY}/p_Y \) specifies the conditional probability that the neighboring site of a state of state \( Y \) is in state \( X \) in equilibrium state of pairwise interaction dynamics. Herein, \( X \) and \( Y \) stand for the state of a site, which is occupied by either an expeller or a cooperator or a defector, or just vacant. For pair approximation method [1–6], only frequencies of state pairs \( p_{XY} \) are tracked. The probabilities of larger configurations are expressed and approximated by the frequencies of pair configurations. Based on the symmetry condition \( p_{XY} = p_Y X \), the compatibility condition \( p_X = \sum_Y p_{XY} \), and the closure conditions, the whole system can be described by the following eight variables in pair approximation: \( p_E, p_C, p_{EE}, p_{EC}, p_{ED}, p_{CC}, p_{CD} \) and \( p_{DD} \). Let us now consider the variations of configuration frequencies induced by a strategy updating event.

1.1 Updating the strategy of a defector

The randomly selected focal defector has \( k_E \) expellers, \( k_C \) cooperators, \( k_D \) defectors and \( k_\phi \) vacant sites \( (k_\phi = k - k_E - k_C - k_D) \) in its neighborhood on a regular graph with connectivity \( k \). The frequency of such a configuration is

\[
\frac{k!}{k_E!k_C!k_D!k_\phi!} q_{q_D}^{k_\phi} \left( 1 - q_D \right)^{k - k_\phi} \frac{(k - k_\phi)!}{k_D!(k - k_\phi - k_D)!} \left( \frac{q_D}{1 - q_D} \right)^{k_D} \left( 1 - \frac{q_D}{1 - q_D} \right)^{k - k_\phi - k_D} \frac{(k_\phi + k_C)!}{k_E!k_C!} \left( \frac{q_E}{q_E + q_C} \right)^{k_E} \left( \frac{q_C}{q_E + q_C} \right)^{k_C}.
\]

As \( w \to 0 \), the expected mean payoff of the focal defector accumulated during pairwise interaction stage can be approximated by \( \tilde{P}_D (k_E, k_C, k_D) = (k_E + k_C)/(k_E + k_C + k_D) \) using the following payoff matrix:

\[
\begin{array}{c|ccc}
 & E & C & D \\
\hline
E & 1 - r & 1 - r & -r \\
C & 1 - r & 1 - r & -r \\
D & 1 & 1 & 0
\end{array}
\]

Similarly, the expected mean payoff of a neighboring expeller is \( \tilde{P}_E (k'_E, k'_C, k'_D) = ((k'_E + k'_C)/(1 - r) + (k'_D + 1)/r - c)/((k'_E + k'_C + k'_D + 1) \cdot c \) where \( c \) is the cost that an expeller pays to exclude a defector, and \( k'_E, k'_C \) and \( k'_D \) is the number of expellers, cooperators and defectors among the \( k - 1 \) remaining neighbors besides the focal defector, respectively. The frequency of this
configuration is
\[
\frac{(k-1)!}{k!} q_{E|D}^k (1 - q_{E|D})^{k-k_E} \\
\times \frac{(k-1-k_E)!}{k!} \frac{q_{C|D}^k}{1 - q_{E|D}} k_C' \left( 1 - \frac{q_{C|D}^k}{1 - q_{E|D}} \right)^{k-1-k_E-k_C'} \\
\times \frac{(k_D'+k_o')!}{k D' k_o!} \frac{q_{D'|D}^k}{q_{D'|D}^k + q_{o|D}^k} k_D' \frac{q_{o|D}^k}{q_{D'|D}^k + q_{o|D}^k} k_o',
\]

where \( q_{X|YZ} \) gives the conditional probability that a site next to the \( YZ \) pair is in state \( X \). Here \( X, Y \) and \( Z \) denote the state of a site, which is occupied by either an expeller or a cooperator or a defector, or just vacant. The probability that the focal defector switches to an expeller can be written as

\[
W_{D\rightarrow E} = \frac{k_E}{k} \sum_{k_E' + k_C' + k_D' + k_o' = k} \frac{(k-1)!}{k!} q_{E|D}^k (1 - q_{E|D})^{k-k_E} \\
\times \frac{(k-1-k_E')!}{k!} \frac{q_{C|D}^k}{1 - q_{E|D}} k_C' \left( 1 - \frac{q_{C|D}^k}{1 - q_{E|D}} \right)^{k-1-k_E'-k_C'} \\
\times \frac{(k_D'+k_o')!}{k D' k_o!} \frac{q_{D'|D}^k}{q_{D'|D}^k + q_{o|D}^k} k_D' \frac{q_{o|D}^k}{q_{D'|D}^k + q_{o|D}^k} k_o'. \tag{S.1}
\]

Consequently, \( p_E \) increases by \( 1/N \) (a defector imitating an expeller), where \( N \) denotes the site size, with probability

\[
\text{Pr} \left( \Delta p_E = \frac{1}{N} \right) = p_D \sum_{k_E+k_C+k_D+k_o=k} \frac{k!}{k_o! (k-k_o)!} q_{o|D}^k (1 - q_{o|D})^{k-k_o} \\
\times \frac{(k-1-k_E)!}{k!} \frac{q_{C|D}^k}{1 - q_{E|D}} k_C' \left( 1 - \frac{q_{C|D}^k}{1 - q_{E|D}} \right)^{k-1-k_E-k_C'} \\
\times \frac{(k_D'+k_o')!}{k D' k_o!} \frac{q_{D'|D}^k}{q_{D'|D}^k + q_{o|D}^k} k_D' \frac{q_{o|D}^k}{q_{D'|D}^k + q_{o|D}^k} k_o'. \tag{S.2}
\]

At the same time, the number of \( EE \) pairs increases by \( k_E \), and thus \( p_{EE} \) increases by \( 2k_E/(kN) \) with probability

\[
\text{Pr} \left( \Delta p_{EE} = \frac{2k_E}{kN} \right) = p_D \frac{k!}{k_E! (k-k_E)!} q_{E|D}^k (1 - q_{E|D})^{k-k_E} \\
\times \frac{(k-1-k_E)!}{k!} \frac{q_{C|D}^k}{1 - q_{E|D}} k_C' \left( 1 - \frac{q_{C|D}^k}{1 - q_{E|D}} \right)^{k-1-k_E-k_C'} \\
\times \frac{(k_D'+k_o')!}{k D' k_o!} \frac{q_{D'|D}^k}{q_{D'|D}^k + q_{o|D}^k} k_D' \frac{q_{o|D}^k}{q_{D'|D}^k + q_{o|D}^k} k_o'. \tag{S.3}
\]

The number of \( EC \) pairs increases by \( k_C \), and thus \( p_{EC} \) increases by \( 2k_C/(kN) \) with probability

\[
\text{Pr} \left( \Delta p_{EC} = \frac{2k_C}{kN} \right) = p_D \frac{k!}{k_C! (k-k_C)!} q_{E|D}^k (1 - q_{E|D})^{k-k_C} \\
\times \frac{(k-1-k_C)!}{k!} \frac{q_{C|D}^k}{1 - q_{E|D}} k_E' \left( 1 - \frac{q_{C|D}^k}{1 - q_{E|D}} \right)^{k-1-k_C-k_E'} \\
\times \frac{(k_D'+k_o')!}{k D' k_o!} \frac{q_{D'|D}^k}{q_{D'|D}^k + q_{o|D}^k} k_D' \frac{q_{o|D}^k}{q_{D'|D}^k + q_{o|D}^k} k_o'. \tag{S.4}
\]
The number of $ED$ pairs increases by $k_D - k_E$, and thus $p_{ED}$ increases by $2(k_D - k_E)/(kN)$ with probability
\[
\Pr_{D\to E} \left( \Delta p_{ED} = \frac{2(k_D - k_E)}{kN} \right) = p_D k_E !(k - k_E) ! q_E^D k_D \left( 1 - \frac{q_D}{1 - q_D} \right) k_D^{-k_E} \times \left( 1 - \frac{q_D}{1 - q_D} \right)^{k_D - k_E} \times \sum_{k_D = 0}^{k_D - k_E} \frac{k_C ! (k_C - k_D - k_E) !}{k_C ! (k_C - k_D - k_E - k_D) !} \frac{q_C}{q_C + q_D}^D \frac{q_D}{q_C + q_D}^D \times W_{D\to E}. \tag{S.5}
\]

The number of $CD$ pairs decreases by $k_C$, and thus $p_{CD}$ decreases by $2k_C/(kN)$ with probability
\[
\Pr_{D\to E} \left( \Delta p_{CD} = -\frac{2k_C}{kN} \right) = p_D k_C !(k - k_C) ! q_C^D k_C \left( 1 - \frac{q_C}{1 - q_C} \right) k_C^{-k_C} \times \left( 1 - \frac{q_C}{1 - q_C} \right)^{k_C - k_E} \times \sum_{k_D = 0}^{k_D - k_E} \frac{k_C ! (k_C - k_D - k_E) !}{k_C ! (k_C - k_D - k_E - k_C) !} \frac{q_C}{q_C + q_D}^D \frac{q_D}{q_C + q_D}^D \times W_{D\to E}. \tag{S.6}
\]

The number of $DD$ pairs decreases by $k_D$, and thus $p_{DD}$ decreases by $2k_D/(kN)$ with probability
\[
\Pr_{D\to E} \left( \Delta p_{DD} = -\frac{2k_D}{kN} \right) = p_D k_D !(k - k_D) ! q_D^D k_D \left( 1 - q_D \right) k_D^{-k_D} \times \left( 1 - q_D \right)^{k_D - k_E} \times \sum_{k_D = 0}^{k_D - k_E} \frac{k_C ! (k_C - k_D - k_E) !}{k_C ! (k_C - k_D - k_E - k_C) !} \frac{q_C}{q_C + q_D}^D \frac{q_D}{q_C + q_D}^D \times W_{D\to E}. \tag{S.7}
\]

Similarly, the probability that $p_C$ increases by $1/N$ (a defector imitating a cooperator) is given by
\[
\Pr_{D\to C} \left( \Delta p_C = \frac{1}{N} \right) = p_D k_C ! (k - k_C) ! \frac{q_C ! (k - k_C) !}{k_C ! (k - k_C) !} q_C^D k_C \left( 1 - \frac{q_C}{1 - q_C} \right) k_C^{-k_C} \times \left( 1 - \frac{q_C}{1 - q_C} \right)^{k_C - k_E} \times \sum_{k_E = 0}^{k_E + k_C + k_D + k_C = k} \frac{k_C ! (k_C - k_D - k_E) !}{k_C ! (k_C - k_D - k_E - k_C) !} \frac{q_C}{q_C + q_D}^D \frac{q_D}{q_C + q_D}^D \times W_{D\to C}, \tag{S.8}
\]

where $W_{D\to C}$ denotes the probability that the focal defector switches to a cooperator, i.e.,
\[
W_{D\to C} = \frac{k_C}{k} \sum_{k_E' + k_C' + k_D' + k_C' = k-1} \frac{(k - 1) !}{k_E ! (k - 1 - k_E) !} \frac{q_C ! (k - 1 - k_E) !}{k_C ! (k - 1 - k_E - k_C) !} \frac{q_C}{q_C + q_D}^D \frac{q_D}{q_C + q_D}^D \times \left( 1 - \frac{q_C}{1 - q_C} \right)^{k_C' - k_D'} \times \left( 1 - \frac{q_C}{1 - q_C} \right)^{k_C' - k_E'} \times \sum_{k_D = 0}^{k_D + k_E' + k_C' + k_D' + k_C' = 0} \frac{k_C' ! (k_C' - k_D' - k_E') !}{k_C' ! (k_C' - k_D' - k_E' - k_C') !} \frac{q_C}{q_C + q_D}^D \frac{q_D}{q_C + q_D}^D \times \left( 1 - \frac{q_C}{1 - q_C} \right)^{k_C' - k_D'} \times \left( 1 - \frac{q_C}{1 - q_C} \right)^{k_C' - k_E'} \times W_{D\to C}. \tag{S.9}
\]
where \( \tilde{P}_C(k_E', k_C', k_D') = \frac{([k_E' + k_C'] (1 - r) + (k_D' + 1) (-r)]/(k_E' + k_C' + k_D' + 1)}{P_D(k_E, k_C, k_D) = (k_E + k_C)/(k_E + k_C + k_D).} \) The number of \( EC \) pairs increases by \( k_E \), and thus \( p_{EC} \) increases by \( 2k_E/(kN) \) with probability

\[
\Pr_{D \rightarrow C}(\Delta p_{EC} = \frac{2k_E}{kN}) = p_D^{k_E}(k_{k-E'}) q_{E|D})^{k_E} (1 - q_{E|D})^{k_{k-E}} \times \sum_{k_{C}=0}^{k_{E}} \frac{(k_{k-E})!}{k_{C}!(k_{k-E}-k_C)!} \left( \frac{q_{C|D}}{1-q_{E|D}} \right)^{k_C} \left( 1 - \frac{q_{C|D}}{1-q_{E|D}} \right)^{k_{-k-E-k_C}} \times \sum_{k_{D}=0}^{k_{k-E-k-C}} \frac{(k_{k-E-k-C})!}{k_{D}!(k_{k-E-k-C}-k_D)!} \left( \frac{q_{D|D}+q_{D|D}}{q_{D|D}+q_{D|D}} \right)^{k_{k-E-k-C-k_D}} \times W_{D \rightarrow C}.
\]

(S.10)

The number of \( ED \) pairs decreases by \( k_E \), and thus \( p_{ED} \) decreases by \( 2k_E/(kN) \) with probability

\[
\Pr_{D \rightarrow C}(\Delta p_{ED} = \frac{-2k_E}{kN}) = p_D^{k_E}(k_{k-E'}) q_{E|D})^{k_E} (1 - q_{E|D})^{k_{k-E}} \times \sum_{k_{C}=0}^{k_{E}} \frac{(k_{k-E})!}{k_{C}!(k_{k-E}-k_C)!} \left( \frac{q_{C|D}}{1-q_{E|D}} \right)^{k_C} \left( 1 - \frac{q_{C|D}}{1-q_{E|D}} \right)^{k_{-k-E-k_C}} \times \sum_{k_{D}=0}^{k_{k-E-k-C}} \frac{(k_{k-E-k-C})!}{k_{D}!(k_{k-E-k-C}-k_D)!} \left( \frac{q_{D|D}+q_{D|D}}{q_{D|D}+q_{D|D}} \right)^{k_{k-E-k-C-k_D}} \times W_{D \rightarrow C}.
\]

(S.11)

The number of \( CC \) pairs increases by \( k_C \), and thus \( p_{CC} \) increases by \( 2k_C/(kN) \) with probability

\[
\Pr_{D \rightarrow C}(\Delta p_{CC} = \frac{2k_C}{kN}) = p_D^{k_E}(k_{k-E'}) q_{E|D})^{k_E} (1 - q_{E|D})^{k_{k-E}} \times \sum_{k_{E}=0}^{k_{k-E}} \frac{(k_{k-E})!}{k_{E}!(k_{k-E}-k_E)!} \left( \frac{q_{E|D}}{1-q_{E|D}} \right)^{k_E} \left( 1 - \frac{q_{E|D}}{1-q_{E|D}} \right)^{k_{-k-E-k_E}} \times \sum_{k_{D}=0}^{k_{k-E-k-C}} \frac{(k_{k-E-k-C})!}{k_{D}!(k_{k-E-k-C}-k_D)!} \left( \frac{q_{D|D}+q_{D|D}}{q_{D|D}+q_{D|D}} \right)^{k_{k-E-k-C-k_D}} \times W_{D \rightarrow C}.
\]

(S.12)

The number of \( CD \) pairs increases by \( k_D - k_C \), and thus \( p_{CD} \) increases by \( 2(k_D - k_C)/(kN) \) with probability

\[
\Pr_{D \rightarrow C}(\Delta p_{CD} = \frac{2(k_D-k_C)}{kN}) = p_D^{k_E}(k_{k-E'}) q_{E|D})^{k_E} (1 - q_{E|D})^{k_{k-E}} \times \sum_{k_{E}=0}^{k_{k-E}} \frac{(k_{k-E})!}{k_{E}!(k_{k-E}-k_E)!} \left( \frac{q_{E|D}}{1-q_{E|D}} \right)^{k_E} \left( 1 - \frac{q_{E|D}}{1-q_{E|D}} \right)^{k_{-k-E-k_E}} \times \sum_{k_{D}=0}^{k_{k-E-k-C}} \frac{(k_{k-E-k-C})!}{k_{D}!(k_{k-E-k-C}-k_D)!} \left( \frac{q_{D|D}+q_{D|D}}{q_{D|D}+q_{D|D}} \right)^{k_{k-E-k-C-k_D}} \times W_{D \rightarrow C}.
\]

(S.13)
The number of $DD$ pairs decreases by $k_D$, and thus $p_{DD}$ decreases by $2k_D/(kN)$ with probability

$$\text{Pr}_{D\rightarrow C} \left( \Delta p_{DD} = \frac{-2k_D}{kN} \right)$$

$$= \frac{k_D}{kD!(k-kD)!}D^D_D \sum_{kE=0}^{kD} \frac{(k-kD)!}{kE!(kD-kE)!} \left( \frac{q_{ED}}{1-q_{ED}} \right)^kE \left( \frac{1-q_{ED}}{1-q_{ED}} \right)^{kD-kE-kE}$$

$$\times \sum_{kC=0}^{kD-kE} \frac{(k-kD-kE)!}{kC!(kD-kE-kC)!} \left( \frac{q_{ED}}{q_{ED}+q_{CD}} \right)^kC \left( \frac{q_{ED}+q_{CD}}{q_{ED}+q_{CD}} \right)^{kD-kE-kC}$$

$$\times W_{D\rightarrow C}. \quad (S.14)$$

1.2 Updating the strategy of a cooperator

The randomly selected focal cooperator has $k_E$ expellers, $k_C$ cooperators, $k_D$ defectors and $k_\phi$ vacant sites ($k_\phi = k-k_E-k_C-k_D$) in its neighborhood. The frequency of such a configuration is

$$\frac{k_D!}{kD!(k-kD)!}D^D_D \left( 1-q_{E|C} \right)^{k-k_\phi} \times \frac{(k-kD)!}{kD!(k-kD-kD)!} \left( \frac{q_{ED}|C}{1-q_{ED}|C} \right)^kD \left( 1 \right) \frac{q_{ED}|C}{1-q_{ED}|C} \times \frac{(kE+kC)!}{kE!kC!} \left( \frac{q_{ED}|C}{q_{ED}|C+q_{CD}|C} \right)^kE \left( \frac{q_{ED}|C+q_{CD}|C}{q_{ED}|C+q_{CD}|C} \right)^kC.$$

The expected mean payoff of the focal cooperator is $\bar{P}_C(k_E,k_C,k_D) = [(k_E + k_C) (1-r) + k_D (-r)]/(k_E + k_C + k_D)$. Similarly, the expected mean payoff of a neighboring expeller is $\bar{P}_E(k_E',k_C',k_D') = [(k_E' + k_C' + 1) (1-r) + k_D' (-r-c)]/(k_E' + k_C' + k_D' + 1)$, where $k_E'$, $k_C'$ and $k_D'$ is the number of expellers, cooperators and defectors among the $k-1$ remaining neighbors besides the focal cooperator, respectively. The frequency of this configuration is

$$\left( \frac{(kE-kE')!}{kE-kE'|kE-kE'|} \right) \left( \frac{q_{ED}|C}{1-q_{ED}|C} \right)^{kE'} \left( 1 \right) \frac{q_{ED}|C}{1-q_{ED}|C} \times \left( \frac{(kC-kC')!}{kC-kC'|kC-kC'|} \right) \left( \frac{q_{ED}|C}{1-q_{ED}|C} \right)^{kE'} \left( 1 \right) \frac{q_{ED}|C}{1-q_{ED}|C} \times \left( \frac{(kD-kD')!}{kD-kD'|kD-kD'|} \right) \left( \frac{q_{ED}|C}{1-q_{ED}|C} \right)^{kE'} \left( 1 \right) \frac{q_{ED}|C}{1-q_{ED}|C}.$$

The probability that the focal cooperator switches to an expeller can be written as

$$W_{C\rightarrow E} = \frac{k_E}{k} \sum_{kE'+kC'+kD'+k_\phi'=k-1} \frac{(k-1)!}{(k-1-kE')!} q_{E|C}^{kE'} \left( 1-q_{E|C} \right)^{kE'} \times \frac{(k-1-kC')!}{(k-1-kC')!} q_{C|E}^{kC'} \left( 1-q_{C|E} \right)^{kC'} \times \frac{(k-1-kD')!}{(k-1-kD')!} q_{D|E}^{kD'} \left( 1-q_{D|E} \right)^{kD'} \times \frac{(k-1-k_\phi')!}{(k-1-k_\phi')!} q_{D|E}^{k_\phi'} \left( 1-q_{D|E} \right)^{k_\phi'} \times kD'! q_{D|E}^{kD'} \left( 1-q_{D|E} \right)^{kD'} \times kD'! q_{D|E}^{kD'} \left( 1-q_{D|E} \right)^{kD'} \times k_\phi'! q_{D|E}^{k_\phi'} \left( 1-q_{D|E} \right)^{k_\phi'} \times q_{E|C}^{kE'} \left( 1-q_{E|C} \right)^{kE'} \times q_{C|E}^{kC'} \left( 1-q_{C|E} \right)^{kC'} \times q_{D|E}^{kD'} \left( 1-q_{D|E} \right)^{kD'} \times q_{D|E}^{k_\phi'} \left( 1-q_{D|E} \right)^{k_\phi'} \times \text{Tr} \left( P_E(k_E',k_C',k_D') - \bar{P}_C(k_E,k_C,k_D) \right). \quad (S.15)$$
Consequently, \( p_E \) increases by \( 1/N \) (a cooperator imitating an expeller) with probability

\[
\text{Prob}_{C \rightarrow E} \left( \Delta p_E = \frac{1}{N} \right) = p_C \sum_{k_E + k_C + k_D + k_E = k} \frac{k_D!}{k_D!} \left( \frac{q_D|C}{1-q_D|C} \right)^{k_D} \left( 1 - \frac{q_D|C}{1-q_D|C} \right)^{k_E-k_D} \times \left( \frac{q_C|E}{q_C|E+q_C|C} \right)^{k_C} \times \left( \frac{q_C}{q_C+q_E} \right)^{k_C} \times W_{C \rightarrow E}.
\]

\( p_C \) decreases by \( 1/N \) (a cooperator imitating an expeller) with the same probability, namely,

\[
\text{Prob}_{C \rightarrow E} \left( \Delta p_C = -\frac{1}{N} \right) = p_C \sum_{k_E + k_C + k_D + k_C = k} \frac{k_D!}{k_D!} \left( \frac{q_D|C}{1-q_D|C} \right)^{k_D} \left( 1 - \frac{q_D|C}{1-q_D|C} \right)^{k_E-k_D} \times \left( \frac{q_C|E}{q_C|E+q_C|C} \right)^{k_C} \times \left( \frac{q_C}{q_C+q_E} \right)^{k_C} \times W_{C \rightarrow E}.
\]

At the same time, the number of \( EE \) pairs increases by \( k_E \), and thus \( p_{EE} \) increases by \( 2k_E/(kN) \) with probability

\[
\text{Prob}_{C \rightarrow E} \left( \Delta p_{EE} = \frac{2k_E}{kN} \right) = p_C \sum_{k_E + k_C + k_D + k_E = k} \frac{k_D!}{k_D!} \left( \frac{q_D|C}{1-q_D|C} \right)^{k_D} \left( 1 - \frac{q_D|C}{1-q_D|C} \right)^{k_E-k_D} \times \left( \frac{q_C|E}{q_C|E+q_C|C} \right)^{k_C} \times \left( \frac{q_C}{q_C+q_E} \right)^{k_C} \times W_{C \rightarrow E}.
\]

The number of \( EC \) pairs increases by \( k_C - k_E \), and thus \( p_{EC} \) increases by \( 2(k_C - k_E)/(kN) \) with probability

\[
\text{Prob}_{C \rightarrow E} \left( \Delta p_{EC} = \frac{2(k_C-k_E)}{kN} \right) = p_C \sum_{k_E + k_C + k_D + k_E = k} \frac{k_D!}{k_D!} \left( \frac{q_D|C}{1-q_D|C} \right)^{k_D} \left( 1 - \frac{q_D|C}{1-q_D|C} \right)^{k_E-k_D} \times \left( \frac{q_C|E}{q_C|E+q_C|C} \right)^{k_C} \times \left( \frac{q_C}{q_C+q_E} \right)^{k_C} \times W_{C \rightarrow E}.
\]

The number of \( ED \) pairs increases by \( k_D \), and thus \( p_{ED} \) increases by \( 2k_D/(kN) \) with probability

\[
\text{Prob}_{C \rightarrow E} \left( \Delta p_{ED} = \frac{2k_D}{kN} \right) = p_C \sum_{k_E + k_C + k_D + k_E = k} \frac{k_D!}{k_D!} \left( \frac{q_D|C}{1-q_D|C} \right)^{k_D} \left( 1 - \frac{q_D|C}{1-q_D|C} \right)^{k_E-k_D} \times \left( \frac{q_C|E}{q_C|E+q_C|C} \right)^{k_C} \times \left( \frac{q_C}{q_C+q_E} \right)^{k_C} \times W_{C \rightarrow E}.
\]
The number of $CC$ pairs decreases by $k_C$, and thus $p_{CC}$ decreases by $2k_C/(kN)$ with probability
\[
\Pr_{C\rightarrow E} \left( \Delta p_{CC} = -\frac{2k_C}{kN} \right) = p_C \frac{k!}{k!(k-k_C)!} q_{E|C}^{k_C} (1 - q_{E|C})^{k-k_C} \\
\times \sum_{k_E=0}^{k-k_C-k_E} \frac{(k-k_C-k_E)!}{k_E!(k-k_C-k_E-k_D)!} \left( \frac{q_{E|C}}{1-q_{E|C}} \right)^{k_E} \left( 1 - \frac{q_{E|C}}{1-q_{E|C}} \right)^{k-k_C-k_E-k_D}
\times \sum_{k_D=0}^{k-k_C-k_E} \frac{(k-k_C-k_E-k_D)!}{k_D!(k-k_C-k_E-k_D)!} \left( \frac{q_{E|C}}{q_{E|C}+q_{E|C}} \right)^{k_D} \left( \frac{q_{E|C}}{q_{E|C}+q_{E|C}} \right)^{k-k_C-k_E-k_D}
\times W_{C\rightarrow E}.
\]
\[(S.21)\]

The number of $CD$ pairs decreases by $k_D$, and thus $p_{CD}$ decreases by $2k_D/(kN)$ with probability
\[
\Pr_{C\rightarrow E} \left( \Delta p_{CD} = -\frac{2k_D}{kN} \right) = p_C \frac{k!}{k!(k-k_D)!} q_{D|C}^{k_D} (1 - q_{D|C})^{k-k_D} \\
\times \sum_{k_C=0}^{k-k_C-k_E} \frac{(k-k_D-k_C)!}{k_C!(k-k_C-k_D)!} \left( \frac{q_{D|C}}{1-q_{D|C}} \right)^{k_C} \left( 1 - \frac{q_{D|C}}{1-q_{D|C}} \right)^{k-k_C-k_E-k_D}
\times \sum_{k_E=0}^{k-k_C-k_D} \frac{(k-k_C-k_D-k_E)!}{k_E!(k-k_C-k_D-k_E)!} \left( \frac{q_{E|C}}{q_{E|C}+q_{E|C}} \right)^{k_E} \left( \frac{q_{E|C}}{q_{E|C}+q_{E|C}} \right)^{k-k_C-k_D-k_E}
\times W_{C\rightarrow E}.
\]
\[(S.22)\]

Similarly, the probability that $p_C$ decreases by $1/N$ (a defector imitating a cooperator) is given by
\[
\Pr_{C\rightarrow D} \left( \Delta p_C = -\frac{1}{N} \right) = p_C \sum_{k_E+k_C+k_D+k_S=k} \frac{k!}{k!(k-k_S)!} q_{E|C}^{k_S} (1 - q_{E|C})^{k-k_S}
\times \frac{(k-k_S)!}{k_D!(k-k_S-k_D)!} \left( \frac{q_{D|C}}{1-q_{D|C}} \right)^{k_D} \left( 1 - \frac{q_{D|C}}{1-q_{D|C}} \right)^{k-k_S-k_D}
\times \frac{(k-k_S-k_D)!}{k_C!(k-k_S-k_D-k_C)!} \left( \frac{q_{C|E}}{1-q_{C|E}} \right)^{k_C} \left( 1 - \frac{q_{C|E}}{1-q_{C|E}} \right)^{k-k_S-k_D-k_C}
\times \frac{(k-k_S-k_D-k_C)!}{k_E!(k-k_S-k_D-k_C-k_E)!} \left( \frac{q_{E|C}}{q_{E|C}+q_{E|C}} \right)^{k_E} \left( \frac{q_{E|C}}{q_{E|C}+q_{E|C}} \right)^{k-k_S-k_D-k_C-k_E}
\times W_{C\rightarrow D},
\]
\[(S.23)\]

where $W_{C\rightarrow D}$ denotes the probability that the focal cooperator switches to a defector, i.e.,
\[
W_{C\rightarrow D} = \frac{k_D}{k} \sum_{k_E'+k_C'+k_D'+k_S'=k-1} \frac{(k-1)!}{k_E'!(k-1-k_E')!} q_{E|D}^{k_E'} (1 - q_{E|D})^{k-1-k_E'}
\times \frac{(k-1-k_E')!}{k_C'!(k-1-k_E'-k_C')!} \left( \frac{q_{C|E}}{1-q_{C|E}} \right)^{k_C'} \left( 1 - \frac{q_{C|E}}{1-q_{C|E}} \right)^{k-1-k_E'-k_C'}
\times \frac{(k-1-k_E'-k_C')!}{k_D'!(k-1-k_E'-k_C'-k_D')!} \left( \frac{q_{D|E}}{q_{D|E}+q_{E|E}} \right)^{k_D'} \left( \frac{q_{D|E}}{q_{D|E}+q_{E|E}} \right)^{k-1-k_E'-k_C'-k_D'}
\times \frac{(k-1-k_E'-k_C'-k_D')!}{k_E!(k-1-k_E'-k_C'-k_D'-k_E)!} \left( \frac{q_{E|E}}{q_{E|E}+q_{E|E}} \right)^{k_E} \left( \frac{q_{E|E}}{q_{E|E}+q_{E|E}} \right)^{k-1-k_E'-k_C'-k_D'-k_E}
\times \times Tr \left( P_D (k_E', k_C', k_D', k_S') - P_C (k_E', k_C', k_D') \right),
\]
\[(S.24)\]

where $P_D (k_E', k_C', k_D') = (k_E' + k_C' + 1)/(k_E' + k_C' + k_D' + 1)$ and $P_C (k_E, k_C, k_D) = [(k_E + k_C)(1 - r) + k_D (-r)]/(k_E + k_C + k_D)$. At the same time, the number of $EC$ pairs decreases by $k_E$, and thus $p_{EC}$ decreases by $2k_E/(kN)$ with probability
\[
\Pr_{C\rightarrow D} \left( \Delta p_{EC} = -\frac{2k_E}{kN} \right) = p_C \frac{k!}{k!(k-k_E)!} q_{E|C}^{k_E} (1 - q_{E|C})^{k-k_E}
\times \sum_{k_C=0}^{k-k_E-k_C} \frac{(k-k_E-k_C)!}{k_C!(k-k_E-k_C-k_D)!} \left( \frac{q_{E|C}}{1-q_{E|C}} \right)^{k_C} \left( 1 - \frac{q_{E|C}}{1-q_{E|C}} \right)^{k-k_E-k_C-k_D}
\times \sum_{k_D=0}^{k-k_E-k_C-k_D} \frac{(k-k_E-k_C-k_D)!}{k_D!(k-k_E-k_C-k_D-k_E)!} \left( \frac{q_{E|C}}{q_{E|C}+q_{E|C}} \right)^{k_D} \left( \frac{q_{E|C}}{q_{E|C}+q_{E|C}} \right)^{k-k_E-k_C-k_D-k_E}
\times W_{C\rightarrow D}.
\]
\[(S.25)\]
The number of ED pairs increases by $k_E$, and thus $p_{EC}$ increases by $2k_E/(kN)$ with probability

$$\Pr_{C\rightarrow D}\left(\Delta p_{ED} = \frac{2k_E}{kN}\right)$$

$$= \frac{k!}{k_E!(k-k_E)!} qE|C^{k_E} \left(1 - qE|C\right)^{k-k_E} \times \sum_{k_C=0}^{k-k_E} \frac{(k-k_E)!}{k_C!(k-k_E-k_C)!} \left(\frac{qC|E}{1-qE|C}\right)^{k_C} \left(1 - \frac{qC|C}{1-qE|C}\right)^{k-k_E-k_C} \times \sum_{k_D=0}^{k-k_E-k_C} \frac{(k-k_E-k_C)!}{k_D!(k-k_E-k_C-k_D)!} \left(\frac{qD|C}{qE|C+qE|C}\right)^{k_D} \left(\frac{qE|C+qE|C}{qE|C+qE|C}\right)^{k-k_E-k_C-k_D}$$

$$\times W_{C\rightarrow D}. \tag{S.26}$$

The number of CC pairs decreases by $k_C$, and thus $p_{CC}$ decreases by $2k_C/(kN)$ with probability

$$\Pr_{C\rightarrow D}\left(\Delta p_{CC} = \frac{-2k_C}{kN}\right)$$

$$= \frac{k!}{k_C!(k-k_C)!} qC|C^{k_C} \left(1 - qC|C\right)^{k-k_C} \times \sum_{k_E=0}^{k-k_C} \frac{(k-k_C)!}{k_E!(k-k_C-k_E)!} \left(\frac{qE|C}{1-qC|C}\right)^{k_E} \left(1 - \frac{qE|C}{1-qC|C}\right)^{k-k_C-k_E} \times \sum_{k_D=0}^{k-k_C-k_E} \frac{(k-k_C-k_E)!}{k_D!(k-k_C-k_E-k_D)!} \left(\frac{qD|C}{qE|C+qE|C}\right)^{k_D} \left(\frac{qE|C+qE|C}{qE|C+qE|C}\right)^{k-k_C-k_E-k_D}$$

$$\times W_{C\rightarrow D}. \tag{S.27}$$

The number of CD pairs increases by $k_C - k_D$, and thus $p_{CD}$ increases by $2(k_C - k_D)/(kN)$ with probability

$$\Pr_{C\rightarrow D}\left(\Delta p_{CD} = \frac{2(k_C-k_D)}{kN}\right)$$

$$= \frac{k!}{k_C!(k-k_C)!} qC|C^{k_C} \left(1 - qC|C\right)^{k-k_C} \times \frac{(k-k_C)!}{k_E!(k-k_C-k_E)!} \left(\frac{qE|C}{1-qC|C}\right)^{k_E} \left(1 - \frac{qE|C}{1-qC|C}\right)^{k-k_C-k_E} \times \frac{(k-k_C-k_E)!}{k_D!(k-k_C-k_E-k_D)!} \left(\frac{qD|C}{qE|C+qE|C}\right)^{k_D} \left(\frac{qE|C+qE|C}{qE|C+qE|C}\right)^{k-k_C-k_E-k_D}$$

$$\times W_{C\rightarrow D}. \tag{S.28}$$

The number of DD pairs increases by $k_D$, and thus $p_{DD}$ increases by $2k_D/(kN)$ with probability

$$\Pr_{C\rightarrow D}\left(\Delta p_{DD} = \frac{2k_D}{kN}\right)$$

$$= \frac{k!}{k_D!(k-k_D)!} qD|D^{k_D} \left(1 - qD|D\right)^{k-k_D} \times \frac{(k-k_D)!}{k_E!(k-k_D-k_E)!} \left(\frac{qE|C}{1-qD|D}\right)^{k_E} \left(1 - \frac{qE|C}{1-qD|D}\right)^{k-k_D-k_E} \times \frac{(k-k_D-k_E)!}{k_C!(k-k_D-k_E-k_C)!} \left(\frac{qC|C}{qC|C+qC|C}\right)^{k_C} \left(\frac{qC|C+qC|C}{qC|C+qC|C}\right)^{k-k_D-k_E-k_C}$$

$$\times W_{C\rightarrow D}. \tag{S.29}$$
1.3 Updating the strategy of an expeller

The randomly selected focal expeller has $k_E$ expellers, $k_C$ cooperators, $k_D$ defectors and $k_\phi$ vacant sites ($k_\phi = k - k_E - k_C - k_D$) in its neighborhood. The frequency of such a configuration is

$$\frac{k!}{k_\phi!(k-k_\phi)!} q_{|E|}^{k_\phi} (1 - q_{|E|})^{k - k_\phi}$$

$$\times \frac{(k-k_\phi)!}{k_D!(k-k_\phi-k_D)!} \left( \frac{q_{|E|}}{1-q_{|E|}} \right)^{k_D} \left( 1 - \frac{q_{|E|}}{1-q_{|E|}} \right)^{k-k_\phi-k_D}$$

$$\times \frac{(k_E + k_C)!}{k_E!(k_C+k_D+k_\phi)!} \left( \frac{q_{|E|}}{q_{E|E} + q_{|C|}} \right)^{k_E} \left( \frac{q_{|C|}}{q_{E|E} + q_{|C|}} \right)^{k_C}.$$ 

The expected mean payoff of the focal expeller is $P_E(k_E, k_C, k_D) = [(k_E + k_C)(1-r) + k_D(-r-c)] / (k_E + k_C + k_D)$. Similarly, the expected mean payoff of a neighboring cooperator is $P_C(k_E', k_C', k_D') = [(k_E + 1 + k_C')(1-r) + k_D'(-r)] / (k_E' + k_C' + k_D' + 1)$, where $k_E'$, $k_C'$ and $k_D'$ is the number of expellers, cooperators and defectors among the $k - 1$ remaining neighbors besides the focal expeller, respectively. The frequency of this configuration is

$$\frac{(k-1)!}{k_E'!(k-1-k_E')!} q_{|E|}^{k_E'} (1 - q_{|E|})^{k-1-k_E'}$$

$$\times \frac{(k-1-k_E')!}{k_C'(k-1-k_E'-k_C')!} \left( \frac{q_{|E|}^{k_E'}}{1-q_{|E|}^{k_E'}} \right)^{k_C'} \left( 1 - \frac{q_{|E|}^{k_E'}}{1-q_{|E|}^{k_E'}} \right)^{k-1-k_E'-k_C'}$$

$$\times \frac{(k_D'+k_C')!}{k_D'!k_C'!} \left( \frac{q_{|E|}}{q_{E|E} + q_{|C|}^{k_E'}} \right)^{k_D'} \left( \frac{q_{|C|}}{q_{E|E} + q_{|C|}^{k_E'}} \right)^{k_C'}.$$ 

The probability that the focal expeller switches to a cooperator can be written as

$$W_{E\to C} = \frac{k_C}{k} \sum_{k_E' + k_C' + k_D' + k_\phi' = k-1} \frac{(k-1)!}{k_E'!(k-1-k_E')!} q_{|E|}^{k_E'} (1 - q_{|E|})^{k-1-k_E'}$$

$$\times \frac{(k-1-k_E')!}{k_C'(k-1-k_E'-k_C')!} \left( \frac{q_{|E|}^{k_E'}}{1-q_{|E|}^{k_E'}} \right)^{k_C'} \left( 1 - \frac{q_{|E|}^{k_E'}}{1-q_{|E|}^{k_E'}} \right)^{k-1-k_E'-k_C'}$$

$$\times \frac{(k_D'+k_C')!}{k_D'!k_C'!} \left( \frac{q_{|E|}}{q_{E|E} + q_{|C|}^{k_E'}} \right)^{k_D'} \left( \frac{q_{|C|}}{q_{E|E} + q_{|C|}^{k_E'}} \right)^{k_C'}.$$ 

$P_E$ decreases by $1/N$ (an expeller imitating a cooperator) with probability, namely,

$$\Pr_{E\to C} \left( \Delta P_E = -\frac{1}{N} \right)$$

$$= p_E \sum_{k_E+k_C+k_D+k_\phi=k} \frac{(k-1)!}{k_E!(k-1-k_E)!} q_{|E|}^{k_E} (1 - q_{|E|})^{k-1-k_E}$$

$$\times \frac{(k-1-k_E)!}{k_D!(k-1-k_E-k_D)!} \left( \frac{q_{|E|}}{1-q_{|E|}} \right)^{k_D} \left( 1 - \frac{q_{|E|}}{1-q_{|E|}} \right)^{k-1-k_E-k_D}$$

$$\times \frac{(k_E+k_C)!}{k_E!k_C!} \left( \frac{q_{|E|}}{q_{E|E} + q_{|C|}} \right)^{k_E} \left( \frac{q_{|C|}}{q_{E|E} + q_{|C|}} \right)^{k_C}.$$

$P_C$ increases by $1/N$ (an expeller imitating a cooperator) with the same probability, namely,

$$\Pr_{E\to C} \left( \Delta P_C = \frac{1}{N} \right)$$

$$= p_E \sum_{k_E+k_C+k_D+k_\phi=k} \frac{(k-1)!}{k_E!(k-1-k_E)!} q_{|E|}^{k_E} (1 - q_{|E|})^{k-1-k_E}$$

$$\times \frac{(k-1-k_E)!}{k_D!(k-1-k_E-k_D)!} \left( \frac{q_{|E|}}{1-q_{|E|}} \right)^{k_D} \left( 1 - \frac{q_{|E|}}{1-q_{|E|}} \right)^{k-1-k_E-k_D}$$

$$\times \frac{(k_E+k_C)!}{k_E!k_C!} \left( \frac{q_{|E|}}{q_{E|E} + q_{|C|}} \right)^{k_E} \left( \frac{q_{|C|}}{q_{E|E} + q_{|C|}} \right)^{k_C}.$$
At the same time, the number of \(EE\) pairs decreases by \(k_E\), and thus \(p_{EE}\) decreases by \(2k_E/(kN)\) with probability
\[
\text{Pr}_{O\rightarrow C} \left( \Delta p_{EE} = -\frac{2k_E}{kN} \right)
\]
\[
= p_E k_D! q_E^k E \frac{k}{k-1} \sum_{k=0}^{k} \frac{(k-k_E)!}{k!} \left( \frac{q_{C|E}}{1-q_{E|E}} \right)^k \frac{1}{1-q_{E|E}}^{k-k_E}
\]
\[
\times \sum_{k=0}^{k} \frac{(k-k_E)!}{k!} \left( \frac{q_{C|E}}{1-q_{E|E}} \right)^k \frac{1}{1-q_{E|E}}^{k-k_E} \times W_{E\rightarrow C}.
\]

The number of \(EC\) pairs increases by \(k_E - k_C\), and thus \(p_{EC}\) increases by \(2(k_E - k_C)/(kN)\) with probability
\[
\text{Pr}_{O\rightarrow C} \left( \Delta p_{EC} = \frac{2(k_E-k_C)}{kN} \right)
\]
\[
= p_E k_D! q_E^k E \frac{k}{k-1} \sum_{k=0}^{k} \frac{(k-k_E)!}{k!} \left( \frac{q_{C|E}}{1-q_{E|E}} \right)^k \frac{1}{1-q_{E|E}}^{k-k_E} \times W_{E\rightarrow C}.
\]

The number of \(ED\) pairs decreases by \(k_D\), and thus \(p_{ED}\) decreases by \(2k_D/(kN)\) with probability
\[
\text{Pr}_{O\rightarrow C} \left( \Delta p_{ED} = -\frac{2k_D}{kN} \right)
\]
\[
= p_E k_D! q_D^k E \frac{k}{k-1} \sum_{k=0}^{k} \frac{(k-k_D)!}{k!} \left( \frac{q_{C|E}}{1-q_{E|E}} \right)^k \frac{1}{1-q_{E|E}}^{k-k_D} \times W_{E\rightarrow C}.
\]

The number of \(CC\) pairs increases by \(k_C\), and thus \(p_{CC}\) increases by \(2k_C/(kN)\) with probability
\[
\text{Pr}_{O\rightarrow C} \left( \Delta p_{CC} = \frac{2k_C}{kN} \right)
\]
\[
= p_E k_D! q_D^k E \frac{k}{k-1} \sum_{k=0}^{k} \frac{(k-k_C)!}{k!} \left( \frac{q_{C|E}}{1-q_{E|E}} \right)^k \frac{1}{1-q_{E|E}}^{k-k_C} \times W_{E\rightarrow C}.
\]

The number of \(CD\) pairs increases by \(k_D\), and thus \(p_{CD}\) increases by \(2k_D/(kN)\) with probability
\[
\text{Pr}_{O\rightarrow C} \left( \Delta p_{CD} = \frac{2k_D}{kN} \right)
\]
\[
= p_E k_D! q_D^k E \frac{k}{k-1} \sum_{k=0}^{k} \frac{(k-k_D)!}{k!} \left( \frac{q_{C|E}}{1-q_{E|E}} \right)^k \frac{1}{1-q_{E|E}}^{k-k_D} \times W_{E\rightarrow C}.
\]
Similarly, the probability that \( p_E \) decreases by 1/\( N \) (an expeller imitating a defector) is given by

\[
\Pr_{O \rightarrow D} \left( \Delta p_E = -\frac{1}{N} \right) = p_E \sum_{k_E+k_C+k_D+\delta_0 = k} \frac{k!}{k_0!(k-k_0)!} q_{E|E}^{k_0} \left( 1 - q_{E|E} \right)^{k-k_0} \times \frac{1}{k_0!(k-k_0-k_\delta)!} q_{D|E}^{k_\delta} \left( 1 - q_{D|E} \right)^{k-k_\delta-k_D} \times W_{O \rightarrow D} \tag{S.38}
\]

where \( W_{O \rightarrow D} \) denotes the probability that the focal cooperator switches to a defector, i.e.,

\[
W_{O \rightarrow D} = \frac{k_D}{k} \sum_{k_E'+k_C'+k_D'=k-1} \frac{(k-1)!}{k_0!(k-1-k_0')!} q_{E|E}^{k_0'} \left( 1 - q_{E|E} \right)^{k-1-k_0'} \times \frac{1}{k_0!(k-1-k_0'-k_C')!} q_{C|E}^{k_C'} \left( 1 - q_{C|E} \right)^{k-1-k_0'-k_C'} \times \frac{1}{k_0!(k-1-k_0'-k_C'-k_D')!} q_{D|E}^{k_D'} \left( 1 - q_{D|E} \right)^{k-1-k_0'-k_C'-k_D'} \times T r \left( P_D \left( k_E', k_C', k_D' \right) - P_E \left( k_E, k_C, k_D \right) \right) \tag{S.39}
\]

where \( P_D \left( k_E', k_C', k_D' \right) = (k_E' + k_C' + 1)/(k_E' + k_C' + k_D' + 1) \) and \( P_E \left( k_E, k_C, k_D \right) = [(k_E + k_C) (1-r) + k_D (-r-c)]/(k_E + k_C + k_D) \). At the same time, the number of \( EE \) pairs decreases by \( k_E \), and thus \( p_{EE} \) decreases by 2\( k_E/(kN) \) with probability

\[
\Pr_{O \rightarrow D} \left( \Delta p_{EE} = -\frac{2k_E}{kN} \right) = p_E \sum_{k_E+k_C+k_D+\delta_0 = k} \frac{k!}{k_0!(k-k_0)!} q_{E|E}^{k_0} \left( 1 - q_{E|E} \right)^{k-k_0} \times \frac{1}{k_0!(k-k_0-k_\delta)!} q_{C|E}^{k_\delta} \left( 1 - q_{C|E} \right)^{k-k_\delta-k_C} \times \frac{1}{k_0!(k-k_0-k_\delta-k_D)!} q_{D|E}^{k_D} \left( 1 - q_{D|E} \right)^{k-k_\delta-k_D} \times W_{O \rightarrow D} \tag{S.40}
\]

The number of \( EC \) pairs decreases by \( k_C \), and thus \( p_{EC} \) decreases by 2\( k_C/(kN) \) with probability

\[
\Pr_{O \rightarrow D} \left( \Delta p_{EC} = -\frac{2k_C}{kN} \right) = p_E \sum_{k_E+k_C+k_D+\delta_0 = k} \frac{k!}{k_0!(k-k_0)!} q_{E|E}^{k_0} \left( 1 - q_{E|E} \right)^{k-k_0} \times \frac{1}{k_0!(k-k_0-k_\delta)!} q_{C|E}^{k_\delta} \left( 1 - q_{C|E} \right)^{k-k_\delta-k_C} \times \frac{1}{k_0!(k-k_0-k_\delta-k_D)!} q_{D|E}^{k_D} \left( 1 - q_{D|E} \right)^{k-k_\delta-k_D} \times W_{O \rightarrow D} \tag{S.41}
\]
The number of $ED$ pairs increases by $k_E - k_D$, and thus $p_{ED}$ increases by $2(k_E - k_D)/(kN)$ with probability
\[
\Pr_{E \rightarrow D} \left( \Delta p_{ED} = \frac{2(k_E - k_D)}{kN} \right) = p_{E \rightarrow D} \frac{k!}{k_E!(k_E - k_D)!} q_{E|E}^{k_E} \left( 1 - q_{E|E} \right)^{k - k_E} \\
\times \frac{(k - k_E)!}{k_D!(k_E - k_D - k_D)!} \left( \frac{q_{D|E}}{1 - q_{E|E}} \right) \left( \frac{1 - q_{E|E}}{1 - q_{D|E}} \right)^{k - k_E - k_D} \\
\times \sum_{k_C = 0}^{k - k_E - k_D} \frac{(k - k_E - k_D)!}{k_C!(k - k_E - k_D - k_C)!} \left( \frac{q_{C|E}}{1 - q_{E|E}} \right)^{k_C} \left( \frac{q_{E|E}}{q_{C|E} + q_{E|E}} \right)^{k_C} \left( \frac{q_{E|E}}{q_{C|E} + q_{E|E}} \right)^{k - k_E - k_D - k_C} \\
\times W_{E \rightarrow D}. \tag{S.42}
\]

The number of $CD$ pairs increases by $k_C$, and thus $p_{CD}$ increases by $2k_C/(kN)$ with probability
\[
\Pr_{E \rightarrow D} \left( \Delta p_{CD} = \frac{2k_C}{kN} \right) = p_{E \rightarrow D} \frac{k!}{k_C!(k_C - k_D)!} q_{C|E}^{k_C} \left( 1 - q_{C|E} \right)^{k - k_C} \\
\times \sum_{k_E = 0}^{k - k_C} \frac{(k - k_C)!}{k_E!(k_C - k_D)!} \left( \frac{q_{C|E}}{1 - q_{O|E}} \right) \left( \frac{1 - q_{E|E}}{1 - q_{C|E}} \right)^{k_E} \left( \frac{q_{E|E}}{q_{C|E} + q_{E|E}} \right)^{k_E} \left( \frac{q_{E|E}}{q_{C|E} + q_{E|E}} \right)^{k - k_C - k_E - k_D} \\
\times W_{E \rightarrow D}. \tag{S.43}
\]

The number of $DD$ pairs increases by $k_D$, and thus $p_{DD}$ increases by $2k_D/(kN)$ with probability
\[
\Pr_{E \rightarrow D} \left( \Delta p_{DD} = \frac{2k_D}{kN} \right) = p_{E \rightarrow D} \frac{k!}{k_D!(k_D - k_E)!} q_{D|E}^{k_D} \left( 1 - q_{D|E} \right)^{k - k_D} \\
\times \sum_{k_E = 0}^{k - k_D} \frac{(k - k_D)!}{k_E!(k_D - k_E)!} \left( \frac{q_{E|E}}{1 - q_{D|E}} \right) \left( \frac{1 - q_{E|E}}{1 - q_{D|E}} \right)^{k_E} \left( \frac{q_{E|E}}{q_{C|E} + q_{E|E}} \right)^{k_E} \left( \frac{q_{E|E}}{q_{C|E} + q_{E|E}} \right)^{k - k_D - k_E - k_C} \\
\times W_{E \rightarrow D}. \tag{S.44}
\]
1.4 Master equations describing strategy updating dynamics

In the limit of large site size $N \to \infty$, we obtain the following differential equation set:

\[
\begin{align*}
\dot{p}_E &= \lim_{N \to \infty} \frac{\Delta p_E}{(1/N)} = \left[ \text{Prob}_{D \to E} \left( \Delta p_E = \frac{k}{N} \right) + \text{Prob}_{C \to E} \left( \Delta p_E = \frac{k}{N} \right) \right. \\
&\quad - \left. \text{Prob}_{E \to C} \left( \Delta p_E = -\frac{k}{N} \right) - \text{Prob}_{E \to D} \left( \Delta p_E = -\frac{k}{N} \right) \right], \\
\dot{p}_C &= \lim_{N \to \infty} \frac{\Delta p_C}{(1/N)} = \left[ \text{Prob}_{D \to C} \left( \Delta p_C = \frac{k}{N} \right) + \text{Prob}_{E \to C} \left( \Delta p_C = \frac{k}{N} \right) \right. \\
&\quad - \left. \text{Prob}_{C \to E} \left( \Delta p_C = -\frac{k}{N} \right) - \text{Prob}_{C \to D} \left( \Delta p_C = -\frac{k}{N} \right) \right], \\
\dot{p}_{EE} &= \lim_{N \to \infty} \frac{\Delta p_{EE}}{(1/N)} = \sum_{k_E=0}^{k} \frac{2kE}{k} \left[ \text{Prob}_{D \to E} \left( \Delta p_{EE} = \frac{2k}{kN} \right) - \text{Prob}_{E \to D} \left( \Delta p_{EE} = -\frac{2k}{kN} \right) \right], \\
\dot{p}_{EC} &= \lim_{N \to \infty} \frac{\Delta p_{EC}}{(1/N)} = \frac{2}{k} \left[ \sum_{k_E=0}^{k} \sum_{k_C=0}^{k-k_E} (k_E - k_C) \text{Prob}_{D \to C} \left( \Delta p_{EC} = \frac{2k}{kN} \right) \right. \\
&\quad + \sum_{k_E=0}^{k} k_E \text{Prob}_{D \to C} \left( \Delta p_{EC} = -\frac{2k}{kN} \right) - \sum_{k_C=0}^{k} k_C \text{Prob}_{E \to D} \left( \Delta p_{EC} = \frac{2k}{kN} \right), \\
\dot{p}_{ED} &= \lim_{N \to \infty} \frac{\Delta p_{ED}}{(1/N)} = \frac{2}{k} \left[ \sum_{k_E=0}^{k} \sum_{k_D=0}^{k-k_E} (k_E - k_D) \text{Prob}_{D \to E} \left( \Delta p_{ED} = \frac{2k}{kN} \right) \right. \\
&\quad + \sum_{k_E=0}^{k} k_E \text{Prob}_{E \to D} \left( \Delta p_{ED} = -\frac{2k}{kN} \right) - \sum_{k_D=0}^{k} k_D \text{Prob}_{C \to E} \left( \Delta p_{ED} = \frac{2k}{kN} \right), \\
\dot{p}_{CC} &= \lim_{N \to \infty} \frac{\Delta p_{CC}}{(1/N)} = \frac{2}{k} \left[ \sum_{k_C=0}^{k} \sum_{k_D=0}^{k-k_C} (k_C - k_D) \text{Prob}_{C \to D} \left( \Delta p_{CD} = \frac{2k}{kN} \right) \right. \\
&\quad + \sum_{k_C=0}^{k} k_C \text{Prob}_{C \to D} \left( \Delta p_{CD} = -\frac{2k}{kN} \right) - \sum_{k_D=0}^{k} k_D \text{Prob}_{C \to E} \left( \Delta p_{CD} = \frac{2k}{kN} \right), \\
\dot{p}_{CD} &= \lim_{N \to \infty} \frac{\Delta p_{CD}}{(1/N)} = \frac{2}{k} \left[ \sum_{k_C=0}^{k} \sum_{k_D=0}^{k-k_C} (k_D - k_C) \text{Prob}_{D \to C} \left( \Delta p_{CD} = \frac{2k}{kN} \right) \right. \\
&\quad + \sum_{k_C=0}^{k} k_C \text{Prob}_{D \to E} \left( \Delta p_{CD} = -\frac{2k}{kN} \right) - \sum_{k_D=0}^{k} k_D \text{Prob}_{E \to D} \left( \Delta p_{CD} = \frac{2k}{kN} \right), \\
\dot{p}_{DD} &= \lim_{N \to \infty} \frac{\Delta p_{DD}}{(1/N)} = \frac{2}{k} \left[ \sum_{k_D=0}^{k} \sum_{k_C=0}^{k-k_D} (k_D - k_C) \text{Prob}_{D \to C} \left( \Delta p_{DD} = \frac{2k}{kN} \right) \right. \\
&\quad + \sum_{k_D=0}^{k} k_D \text{Prob}_{D \to E} \left( \Delta p_{DD} = -\frac{2k}{kN} \right) - \sum_{k_C=0}^{k} k_C \text{Prob}_{E \to D} \left( \Delta p_{DD} = \frac{2k}{kN} \right). \\
\end{align*}
\]

The above equation set requires a ‘moment closure’ by approximating $q_X|Y \approx q_X|Y$ to describe strategy updating dynamics. Together with equations (B.17)-(B.19) in main text, equation (S.45) can fully describe the evolutionary dynamics of the whole system when $w \to 0$. 

(S.45)
Supplementary References

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