Supplementary Information

for

The effect of parity violation on kinetic models of chiral autocatalyis

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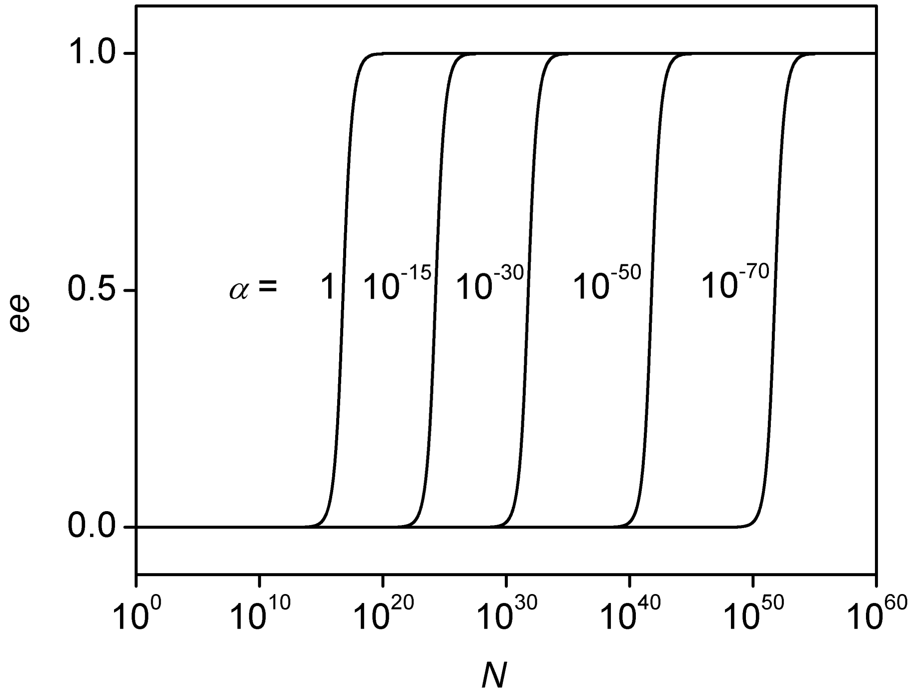

Fig. S1. Curves calculated for the solution of eqn (7) by the deterministic approach for second-order autocatalysis.

Table S1: Wilcoxon rank sum test for the random generation of enantiomers in the Soai-reaction.[63]

x_R	*rank*	x_R	rank	x_R	rank
0.01	1	0.115	36.5	0.77	103.5
0.035	3.5	0.12	39.5	0.775	105
0.035	3.5	0.125	41.5	0.785	106.5
0.04	7	0.13	43	0.79	108
0.04	7	0.14	45.5	0.8	109
0.04	7	0.16	49.5	0.805	110
0.04	7	0.17	55.5	0.83	113.5
0.045	10.5	0.175	58	0.83	113.5
0.045	10.5	0.215	62.5	0.83	113.5
0.05	13	0.24	67	0.835	117
0.05	13	0.27	69	0.835	117
0.05	13	0.31	71	0.835	117
0.055	15	0.315	72	0.84	119.5
0.06	17.5	0.37	74.5	0.855	121.5
0.06	17.5	0.44	80.5	0.855	121.5
0.06	17.5	0.445	82	0.86	123.5
0.06	17.5	0.455	83	0.865	125
0.065	20.5	0.52	85	0.875	127.5
0.075	22.5	0.56	88.5	0.88	129.5
0.08	25	0.565	90	0.885	132.5
0.08	25	0.57	91	0.9	136.5
0.085	27	0.61	92	0.915	141
0.09	30.5	0.615	93	0.915	141
0.09	30.5	0.63	94.5	0.92	144
0.1	32.5	0.68	96	0.925	146.5
0.11	34	0.725	99	0.935	148.5
0.115	36.5	0.75	101	0.96	162
0.115	36.5	0.77	103.5	0.97	167

Sum of ranks: $\sum rank = 6086$

$$W_{84,84} = \sum rank - \frac{84 \times 85}{2} = 2516 \qquad M(W) = 84 \times 84/2 = 3528$$

$$D(W) = \sqrt{\frac{84 \times 84 \times (84 + 84 + 1)}{12}} \approx 315$$

$\left| \frac{W_{84,84} - M(W)}{D(W)} \right| \approx 3.21$ This is larger than the 95% limit (1.96), consequently, the asymmetry in the distribution is significant.

Mathematical proofs for equations appearing in the manuscript

Equation (1):

The Eyring equation gives the rate constant of a reaction as:

$$k = \frac{k_B T}{h} e^{-\Delta G^{\ddagger} / RT} \qquad \text{(S1)}$$

Applying this equation twice to calculate the ratio of the rat constants (k_R/k_S) of the two reactions leading to enantiomers R and S:

$$\frac{k_R}{k_S} = \frac{0.5+\varepsilon}{0.5-\varepsilon} = e^{\Delta E^{\ddagger}{}_{PV} / RT} \qquad \text{(S2)}$$

An approximation for the exponential function from the Taylor series is given by:

$$e^{\Delta E^{\ddagger}{}_{PV} / RT} \approx 1 + \Delta E^{\ddagger}{}_{PV} / RT \qquad \text{(S3)}$$

Using eqn (S3) to modify eqn (S2) gives:

$$\varepsilon = \frac{e^{\Delta E^{\ddagger}{}_{PV} / RT} - 1}{2(e^{\Delta E^{\ddagger}{}_{PV} / RT} + 1)} \approx \frac{1 + \Delta E^{\ddagger}{}_{PV} / RT - 1}{2(1 + \Delta E^{\ddagger}{}_{PV} / RT + 1)} = \frac{\Delta E^{\ddagger}{}_{PV}}{4RT} \qquad \text{(S4)}$$

Equation (7):

Using the new variables and parameters defined in the text transforms the simultaneous differential equations in eqn (5) as follows:

$$\frac{db}{dt} = \kappa_u a + \kappa_c a(r^\xi + s^\xi)$$
$$\frac{dr}{dt} = (0.5+\varepsilon)\kappa_u a + \kappa_c a r^\xi \qquad \text{(S5)}$$
$$\frac{ds}{dt} = (0.5-\varepsilon)\kappa_u a + \kappa_c a s^\xi$$

The definition of Δ can be transformed into :

$$\Delta = ([B_R] - [B_S])VN_A = r - s \qquad \text{(S6)}$$

Differentiating eqn (S6) gives:

$$\frac{d\Delta}{dt} = \frac{dr}{dt} - \frac{ds}{dt} = 2\varepsilon\kappa_u a + \kappa_c a(r^\xi - s^\xi) = 2\varepsilon\kappa_u a + \kappa_c a\left(\frac{b+\Delta}{2}\right)^\xi - \kappa_c a\left(\frac{b-\Delta}{2}\right)^\xi \qquad \text{(S7)}$$

From eqn (S5)

$$\frac{db}{dt} = \kappa_u a + \kappa_c a\left(\frac{b+\Delta}{2}\right)^\xi + \kappa_c a\left(\frac{b-\Delta}{2}\right)^\xi \qquad \text{(S8)}$$

According to the rules of differentiating (http://mathworld.wolfram.com/Derivative.html), the derivative on the left-hand side of eqn (7) can be calculated as:

$$\frac{d\Delta}{db} = \frac{d\Delta}{dt} \bigg/ \frac{db}{dt} \qquad \text{(S9)}$$

Applying eqn (S9) on eqn (S7) and eqn (S8) gives eqn (7).

Equation (8):

Any given (*r*,*s*) state can only arise from either one of the (*r*,*s+1*) and (*r*,*s+1*) states. The probability of state (*r*,*s*) being followed by state (*r*,*s+1*) is (i.e. a B_S molecule forms next):

$$\frac{\kappa_u(0.5-\varepsilon)a+\kappa_c a s^{\xi}}{\kappa_u(0.5-\varepsilon)a+\kappa_c a s^{\xi}+\kappa_u(0.5+\varepsilon)a+\kappa_c a r^{\xi}}=\frac{(0.5-\varepsilon)+\alpha s^{\xi}}{1+\alpha(s^{\xi}+r^{\xi})} \qquad \text{(S10)}$$

Similarly, the probability of (*r*,*s*) being followed by state (*r*+1,*s*) is (i.e. a B_R molecule forms next):

$$\frac{\kappa_u(0.5-\varepsilon)a+\kappa_c a s^{\xi}}{\kappa_u(0.5-\varepsilon)a+\kappa_c a s^{\xi}+\kappa_u(0.5+\varepsilon)a+\kappa_c a r^{\xi}}=\frac{(0.5+\varepsilon)+\alpha r^{\xi}}{1+\alpha(s^{\xi}+r^{\xi})} \qquad \text{(S11)}$$

These formulas are general, they can be used for every state. State (*r*,*s*) can only be formed from in two ways: from state (*r*–1,*s*) through the formation of a B_R molecule and from state (*r*,*s*–1) through the formation of a B_S molecule. Therefore, the probability of the system ever going through state (*r*,*s*) can be calculated from probabilities *Q*(*r*–1,*s*) and *Q*(*r*,*s*–1):

$$Q(r,s)=\frac{(0.5+\varepsilon)+\alpha(r-1)^{\xi}}{1+\alpha\{(r-1)^{\xi}+s^{\xi}\}}Q(r-1,s)+\frac{(0.5-\varepsilon)+\alpha(s-1)^{\xi}}{1+\alpha\{r^{\xi}+(s-1)^{\xi}\}}Q(r,s-1) \qquad (8)$$

Equation (9):

Mathematical induction will be used to prove the formula. The first few values of Q can be calculated using eqn (8):

$$Q(0,0) = 1$$
$$Q(1,0) = 0.5 + \varepsilon \tag{S12}$$
$$Q(0,1) = 0.5 - \varepsilon$$

It is seen that eqn (9) is true for r = 1 and s =1. If the formula is already proved for $r = k$, $Q(k,0)$ can be given as:

$$Q(k,0) = \prod_{i=0}^{k-1} \frac{0.5 + \varepsilon + \alpha i^{\xi}}{1 + \alpha i^{\xi}} \tag{S13}$$

$Q(k+1,0)$ can be calculated using eqn (8). Since s = 0, the second additive term in the eqn (8) can be disregarded.

$$Q(k+1,0) = \frac{(0.5+\varepsilon) + \alpha k^{\xi}}{1 + \alpha\{k^{\xi} + 0^{\xi}\}} Q(k,0) = \frac{(0.5+\varepsilon) + \alpha k^{\xi}}{1 + \alpha k^{\xi}} \prod_{i=0}^{k-1} \frac{0.5 + \varepsilon + \alpha i^{\xi}}{1 + \alpha i^{\xi}} = \prod_{i=0}^{k} \frac{0.5 + \varepsilon + \alpha i^{\xi}}{1 + \alpha i^{\xi}} \tag{S14}$$

Therefore, the first part of eqn (9) is true for all positive integers. An entirely analogous way of thought proves the second part of eqn (9).

Equations (12) and (13):

The first parts of eqn (12) and eqn (13) give the definitions of $R(2k+1)$ and $R(2k+2)$.
Using eqn (8) in the defining part of eqn (13) gives:

$$R(2k+2)=\sum_{i=0}^{k}\left(Q(2k+2-i,i)-Q(i,2k+2-i)\right)=$$

$$\sum_{i=0}^{k}\left(\frac{(0.5+\varepsilon)+\alpha(2k+1-i)^{\xi}}{1+\alpha\{(2k+1-i)^{\xi}+i^{\xi}\}}Q(2k+1-i,i)+\frac{(0.5-\varepsilon)+\alpha(i-1)^{\xi}}{1+\alpha\{(2k+2-i)^{\xi}+(i-1)^{\xi}\}}Q(2k+2-i,i-1)\right)$$
$$-\sum_{i=0}^{k}\left(\frac{(0.5+\varepsilon)+\alpha(i-1)^{\xi}}{1+\alpha\{(i-1)^{\xi}+(2k+2-i)^{\xi}\}}Q(i-1,2k+2-i)+\frac{(0.5-\varepsilon)+\alpha(2k+1-i)^{\xi}}{1+\alpha\{i^{\xi}+(2k+1-i)^{\xi}\}}Q(i,2k+1-i)\right)=$$

$$=\sum_{i=0}^{k}\left(\frac{(0.5+\varepsilon)+\alpha(2k+1-i)^{\xi}}{1+\alpha\{(2k+1-i)^{\xi}+i^{\xi}\}}Q(2k+1-i,i)\right)+\sum_{i=0}^{k-1}\left(\frac{(0.5-\varepsilon)+\alpha i^{\xi}}{1+\alpha\{(2k+1-i)^{\xi}+i^{\xi}\}}Q(2k+1-i,i)\right)$$
$$-\sum_{i=0}^{k-1}\left(\frac{(0.5+\varepsilon)+\alpha i^{\xi}}{1+\alpha\{i^{\xi}+(2k+1-i)^{\xi}\}}Q(i,2k+1-i)\right)-\sum_{i=0}^{k}\left(\frac{(0.5-\varepsilon)+\alpha(2k+1-i)^{\xi}}{1+\alpha\{i^{\xi}+(2k+1-i)^{\xi}\}}Q(i,2k+1-i)\right)=$$

$$=\sum_{i=0}^{k-1}Q(2k+1-i,i)+\frac{(0.5+\varepsilon)+\alpha(k+1)^{\xi}}{1+\alpha\{(k+1)^{\xi}+k^{\xi}\}}Q(k+1,k)-\sum_{i=0}^{k-1}Q(i,2k+1-i)-\frac{(0.5-\varepsilon)+\alpha(k+1)^{\xi}}{1+\alpha\{k^{\xi}+(k+1)^{\xi}\}}Q(k,k+1)=$$

$$=\sum_{i=0}^{k-1}\left(Q(2k+1-i,i)-Q(i,2k+1-i)\right)+\left(1-\frac{(0.5-\varepsilon)+\alpha k^{\xi}}{1+\alpha\{(k+1)^{\xi}+k^{\xi}\}}\right)Q(k+1,k)-\left(1-\frac{(0.5+\varepsilon)+\alpha k^{\xi}}{1+\alpha\{(k+1)^{\xi}+k^{\xi}\}}\right)Q(k,k+1)= \quad \text{(S15)}$$

$$=\sum_{i=0}^{k}\left(Q(2k+1-i,i)-Q(i,2k+1-i)\right)-\frac{(0.5-\varepsilon)+\alpha k^{\xi}}{1+\alpha\{(k+1)^{\xi}+k^{\xi}\}}Q(k+1,k)+\frac{(0.5+\varepsilon)+\alpha k^{\xi}}{1+\alpha\{(k+1)^{\xi}+k^{\xi}\}}Q(k,k+1)$$

It will be shown that the sum of the second and third terms in the last line of eqn (S15) is exactly 0. The formation of exactly one B_R or B_S molecule will be called an R or S step, respectively. A path to a state (r,s) is defined as one particular series steps resulting in the final formation of state (r,s). A path to a state (r,s) therefore contains exactly r R steps and exactly s S steps.

State $(k+1,k)$ can be formed in Θ different paths where

$$\Theta=\binom{2k+1}{k} \quad \text{(S16)}$$

A path is represented by a $(2k+2)$-membered series m, where m_i gives the number of R step after step i. Obviously, $m_0 = 0$, $m_{2k+1} = k+1$ and $m_i \le m_{i+1}$. The probability of one path is given by:

$$P_{m_0 m_1 m_2 \cdots m_{2k+1}}=\prod_{i=0}^{2k}\frac{\aleph}{1+\alpha m_i^{\ \xi}+\alpha(i-m_i)^{\xi}} \quad \text{(S17)}$$

where

$$\aleph = (0.5 + \varepsilon + \alpha m_i^{\ \xi}) \quad \text{if} \quad m_{i+1} > m_i$$
$$\aleph = (0.5 - \varepsilon + \alpha (i - m_i)^{\xi} \quad \text{if} \quad m_{i+1} = m_i \tag{S18}$$

Out of (2*k*+1) overall steps, there are (*k*+1) R steps and *k* S steps. Therefore

$$\prod_{i=0}^{2k} \aleph = (0.5 + \varepsilon + \alpha k^{\xi}) \prod_{i=0}^{k-1} \left[(0.5 + \varepsilon + \alpha i^{\xi})(0.5 - \varepsilon + \alpha i^{\xi}) \right] \tag{S19}$$

A new parameter is introduced next:

$$\Re_{m_0 m_1 m_2 \cdots m_{2k+1}} = \prod_{i=0}^{2k} \frac{1}{1 + \alpha m_i^{\ \xi} + \alpha (i - m_i)^{\xi}} \left(= \prod_{i=1}^{2k} \frac{1}{1 + \alpha m_i^{\ \xi} + \alpha (i - m_i)^{\xi}} \right) \tag{S20}$$

Using this new parameter in calculating *Q*(*k*+*1*,*k*) gives:

$$Q(k+1,k) = \sum_{\text{all } \Theta \text{ paths}} P_{m_0 m_1 m_2 \cdots m_{2k+1}} =$$

$$= \sum_{\text{all } \Theta \text{ paths}} (0.5 + \varepsilon + \alpha k^{\xi}) \prod_{i=0}^{k-1} (0.5 + \varepsilon + \alpha i^{\xi})(0.5 - \varepsilon + \alpha i^{\xi}) \Re_{m_0 m_1 m_2 \cdots m_{2k+1}} = \tag{S21}$$

$$= (0.5 + \varepsilon + \alpha k^{\xi}) \prod_{i=0}^{k-1} \left[(0.5 + \varepsilon + \alpha i^{\xi})(0.5 - \varepsilon + \alpha i^{\xi}) \right] \times \sum_{\text{all } \Theta \text{ paths}} \Re_{m_0 m_1 m_2 \cdots m_{2k+1}}$$

The very same line of reasoning for symmetric state (*k*,*k*+1) gives:

$$Q(k, k+1) = (0.5 - \varepsilon + \alpha k^{\xi}) \prod_{i=0}^{k-1} \left[(0.5 + \varepsilon + \alpha i^{\xi})(0.5 - \varepsilon + \alpha i^{\xi}) \right] \times \sum_{\text{all } \Theta \text{ paths}} \Re_{m_1 m_2 m_3 \cdots m_{2k+1}} \tag{S22}$$

Dividing eqn (S22) with eqn (S21) gives:

$$\frac{(0.5 - \varepsilon) + \alpha k^{\xi}}{(0.5 + \varepsilon) + \alpha k^{\xi}} = \frac{Q(k, k+1)}{Q(k+1, k)} \tag{S23}$$

Rearranging eqn (S23) shows that the second and third terms in the last line of eqn (S15) is exactly 0. Eqn (S15) is therefore transformed into the following formula:

$$R(2k+2) = \sum_{i=0}^{k} \left(Q(2k+1-i, i) - Q(i, 2k+1-i) \right) = R(2k+1) \tag{S24}$$

This proves the non-defining part of eqn (13).

The non-defining part of eqn (12) will be proved through a similar series of algebraic steps. First, using eqn (8) in the defining part of eqn (12) gives:

$$R(2k+1)=\sum_{i=0}^{k}\left(Q(2k+1-i,i)-Q(i,2k+1-i)\right)=$$

$$=\sum_{i=0}^{k}\left(\frac{(0.5+\varepsilon)+\alpha(2k-i)^{\xi}}{1+\alpha\{(2k+1-i)^{\xi}+i^{\xi}\}}Q(2k-i,i)+\frac{(0.5-\varepsilon)+\alpha(i-1)^{\xi}}{1+\alpha\{(2k+1-i)^{\xi}+(i-1)^{\xi}\}}Q(2k+1-i,i-1)\right)$$

$$-\sum_{i=0}^{k}\left(\frac{(0.5+\varepsilon)+\alpha(i-1)^{\xi}}{1+\alpha\{(i-1)^{\xi}+(2k+1-i)^{\xi}\}}Q(i-1,2k+1-i)+\frac{(0.5-\varepsilon)+\alpha(2k-i)^{\xi}}{1+\alpha\{i^{\xi}+(2k-i)^{\xi}\}}Q(i,2k-i)\right)=$$

$$=\sum_{i=0}^{k}\left(\frac{(0.5+\varepsilon)+\alpha(2k-i)^{\xi}}{1+\alpha\{(2k-i)^{\xi}+i^{\xi}\}}Q(2k-i,i)\right)+\sum_{i=0}^{k-1}\left(\frac{(0.5-\varepsilon)+\alpha i^{\xi}}{1+\alpha\{(2k-i)^{\xi}+i^{\xi}\}}Q(2k-i,i)\right)$$

$$-\sum_{i=0}^{k-1}\left(\frac{(0.5+\varepsilon)+\alpha i^{\xi}}{1+\alpha\{i^{\xi}+(2k-i)^{\xi}\}}Q(i,2k-i)\right)-\sum_{i=0}^{k}\left(\frac{(0.5-\varepsilon)+\alpha(2k-i)^{\xi}}{1+\alpha\{i^{\xi}+(2k-i)^{\xi}\}}Q(i,2k-i)\right)=$$

$$=\sum_{i=0}^{k-1}Q(2k-i,i)+\frac{(0.5+\varepsilon)+\alpha k^{\xi}}{1+\alpha\{k^{\xi}+k^{\xi}\}}Q(k,k)-\sum_{i=0}^{k-1}Q(i,2k-i)-\frac{(0.5-\varepsilon)+\alpha k^{\xi}}{1+\alpha\{k^{\xi}+k^{\xi}\}}Q(k,k)=$$

(S25)

$$=\sum_{i=0}^{k}\left(Q(2k-i,i)-Q(i,2k-i)\right)+\frac{2\varepsilon}{1+2\alpha k^{\xi}}Q(k,k)=R(2k)+\frac{2\varepsilon}{1+2\alpha k^{\xi}}Q(k,k)=R(2k-1)+\frac{2\varepsilon Q(k,k)}{1+2\alpha k^{\xi}}$$

This gives a recursive method to calculate R(2k+1) values. As $R(1) = 2\varepsilon$ and $Q(0,0) = 1$, the recursive definition can be rewritten as

$$R(2k+1)=2\varepsilon\sum_{i=0}^{k}\frac{Q(i,i)}{1+2\alpha i^{\xi}} \qquad \text{(S26)}$$

This is exactly the non-defining part of eqn (12).

Equation (14):

The first part of the equation gives the definition of $E(2k+1)$. The second part is proved by the following trivial rearrangements:

$$E(2k+1)=\sum_{i=0}^{k}\frac{2k+1-2i}{2k+1}\big(Q(2k+1-i,i)+Q(i,2k+1-i)\big)=$$

$$=\sum_{i=0}^{k}\left(1-\frac{2i}{2k+1}\right)\big(Q(2k+1-i,i)+Q(i,2k+1-i)\big)=$$

$$=\sum_{i=0}^{k}\big(Q(2k+1-i,i)+Q(i,2k+1-i)\big)-\sum_{i=0}^{k}\frac{2i}{2k+1}\big(Q(2k+1-i,i)+Q(i,2k+1-i)\big)= \tag{S27}$$

$$=\sum_{i=0}^{2k+1}Q(2k+1-i,i)-\sum_{i=0}^{k}\frac{2i}{2k+1}\big(Q(2k+1-i,i)+Q(i,2k+1-i)\big)=$$

In the first term of this equation, the sum involves all the states where the sum of the number of B_R and B_S molecules is exactly $2k+1$. Evidently, the system must go through exactly on of these states, therefore the the sum is 1.

$$\sum_{i=0}^{2k+1}Q(2k+1-i,i)=1 \tag{S28}$$

A combination of eqn (S27) and eqn S(28) gives the non-defining part of eqn (14).

Equation (19):

Eqn(7) takes a much simpler for first-order autocatalysis ($\xi = 1$)

$$\frac{d\Delta}{db} = \frac{2\varepsilon + \alpha\Delta}{1+\alpha b} \tag{S29}$$

After separation of variables and integration:

$$\frac{1}{\alpha}\ln(2\varepsilon + \alpha\Delta) = \frac{1}{\alpha}\ln(1+\alpha b) + D \tag{S30}$$

where D is an integration constant depending on the initial conditions. Initially, $b = 0$ and $\Delta = 0$. The value of D is therefore $\ln(2\varepsilon)/\alpha$. Substituting this value into the eqn (S30):

$$2\varepsilon + \alpha\Delta = 2\varepsilon(1 + \alpha b) \tag{S31}$$

Eqn (19) follows from a simple rearrangement of eqn (S31).

Equation (20):

By simple calculation:

$$x_R = \frac{r}{b} = \frac{r - s + r + s}{b} = \frac{\Delta + b}{2b} = \frac{2\varepsilon b + b}{2b} = 0.5 + \varepsilon \tag{S32}$$

Similarly, using the definition of *ee* gives:

$$ee = |\Delta|/b = 2\varepsilon b/b = 2\varepsilon \tag{S33}$$

Equation (21):

Special cases r = 0 and s = 0 have already been dealt with in eqn (9).
Mathematical induction will be used to show that the equation is correct. The first few values of Q(r,s) can be calculated from the definition and the recursive formula given in eqn (8)

$Q(0,0) = 1$

$Q(1,0) = 0.5 + \varepsilon$

$Q(0,1) = 0.5 - \varepsilon$

$$Q(2,0) = \frac{(0.5+\varepsilon)}{1}\frac{(0.5+\varepsilon)+\alpha}{1+\alpha} \tag{S34}$$

$$Q(1,1) = 2\frac{(0.5+\varepsilon)}{1}\frac{(0.5-\varepsilon)}{1+\alpha}$$

$$Q(2,0) = \frac{(0.5-\varepsilon)}{1}\frac{(0.5-\varepsilon)+\alpha}{1+\alpha}$$

It is seen that eqn (21) is correct for all these cases. If eqn (21) is already proved for $Q(r-1,s)$ and $Q(r,s-1)$, recursive formula eqn (8) can be transformed as follows:

$$Q(r,s) = \frac{(0.5+\varepsilon)+\alpha(r-1)}{1+\alpha\{r-1+s\}}\binom{r+s-1}{r-1}\frac{\prod_{i=0}^{r-2}(0.5+\varepsilon+\alpha i)\prod_{i=0}^{s-1}(0.5-\varepsilon+\alpha i)}{\prod_{i=0}^{r+s-2}(1+\alpha i)}$$

$$+\frac{(0.5-\varepsilon)+\alpha(s-1)}{1+\alpha\{r+(s-1)\}}\binom{r+s-1}{r}\frac{\prod_{i=0}^{r-1}(0.5+\varepsilon+\alpha i)\prod_{i=0}^{s-2}(0.5-\varepsilon+\alpha i)}{\prod_{i=0}^{r+s-2}(1+\alpha i)} =$$

$$=\binom{r+s-1}{r-1}\frac{\prod_{i=0}^{r-1}(0.5+\varepsilon+\alpha i)\prod_{i=0}^{s-1}(0.5-\varepsilon+\alpha i)}{\prod_{i=0}^{r+s-1}(1+\alpha i)}+\binom{r+s-1}{r}\frac{\prod_{i=0}^{r-1}(0.5+\varepsilon+\alpha i)\prod_{i=0}^{s-1}(0.5-\varepsilon+\alpha i)}{\prod_{i=0}^{r+s-1}(1+\alpha i)} =$$

$$=\left\{\binom{r+s-1}{r-1}+\binom{r+s-1}{r}\right\}\frac{\prod_{i=0}^{r-1}(0.5+\varepsilon+\alpha i)\prod_{i=0}^{s-1}(0.5-\varepsilon+\alpha i)}{\prod_{i=0}^{r+s-1}(1+\alpha i)} = \tag{S35}$$

$$=\binom{r+s}{r}\frac{\prod_{i=0}^{r-1}(0.5+\varepsilon+\alpha i)\prod_{i=0}^{s-1}(0.5-\varepsilon+\alpha i)}{\prod_{i=0}^{r+s-1}(1+\alpha i)}$$

Therefore, eqn (21) is true for all positive integers.

Equation (22):

Mathematical induction will be used to show that the equation is correct.

$$\overline{x_R}(1) = 0 \times Q(0,1) + 1 \times Q(1,0) = 0.5 + \varepsilon \tag{S36}$$

It is seen that eqn (22) is correct for b = 1. If eqn (22) is already proved for k, defining eqn (10) and the recursive formula in eqn (8) can be transformed as follows:

$$\overline{x_R}(k+1) = \sum_{i=0}^{k+1} \frac{i}{k+1} Q(i, k+1-i) =$$

$$= \sum_{i=0}^{k+1} \frac{i}{k+1} \left[\frac{(0.5+\varepsilon) + \alpha(i-1)}{1+\alpha\{i-1+k+1-i\}} Q(i-1, k+1-i) + \frac{(0.5-\varepsilon) + \alpha(k-i)}{1+\alpha\{i+k-i\}} Q(i, k-i) \right] =$$

$$= \frac{1}{k+1} \sum_{i=1}^{k+1} iQ(i-1, k+1-i) \frac{(0.5+\varepsilon) + \alpha(i-1)}{1+\alpha k} + \frac{1}{k+1} \sum_{i=0}^{k} iQ(i, k-i) \frac{(0.5-\varepsilon) + \alpha(k-i)}{1+\alpha k} =$$

$$= \frac{1}{k+1} \sum_{i=0}^{k} (i+1) Q(i, k-i) \frac{(0.5+\varepsilon) + \alpha i}{1+\alpha k} + \frac{1}{k+1} \sum_{i=0}^{k} iQ(i, k-i) \frac{(0.5-\varepsilon) + \alpha(k-i)}{1+\alpha k} =$$

$$= \frac{1}{k+1} \sum_{i=0}^{k} iQ(i, k-i)) + \frac{1}{k+1} \sum_{i=0}^{k} Q(i, k-i) \frac{(0.5+\varepsilon) + \alpha i}{1+\alpha k} =$$

$$= \frac{k(0.5+\varepsilon)}{k+1} + \frac{1}{k+1} \sum_{i=0}^{k} Q(i, k-i) \frac{0.5+\varepsilon}{1+\alpha k} + \frac{1}{k+1} \sum_{i=0}^{k} Q(i, k-i) \frac{\alpha i}{1+\alpha k} =$$

$$= \frac{k(0.5+\varepsilon)}{k+1} + \frac{0.5+\varepsilon}{(k+1)(1+\alpha k)} + \frac{\alpha k(0.5+\varepsilon)}{(k+1)(1+\alpha k)} = \tag{S37}$$

$$(0.5+\varepsilon) \frac{k(1+\alpha k) + 1 + \alpha k}{(k+1)(1+\alpha k)} = (0.5+\varepsilon) \frac{k+1}{k+1} = 0.5 + \varepsilon$$

Therefore, eqn (22) is true for all positive integers.

Equation (23):

Mathematical induction will be used to show that the equation is correct.

$$\sigma(1) = \sqrt{\sum_{i=0}^{1}\left(\frac{i^2}{1^2}Q(i,1-i)\right) - \overline{x_R}^2(1)} = \sqrt{0.5+\varepsilon-(0.5+\varepsilon)^2} = \sqrt{(0.5+\varepsilon)(0.5-\varepsilon)} =$$

$$= \sqrt{(0.5+\varepsilon)(0.5-\varepsilon)\frac{1^{-1}+\alpha}{1+\alpha}} \qquad \text{(S38)}$$

It is seen that eqn (23) is correct for b = 1. If eqn (23) is already proved for k, defining eqn (11) and the recursive formula in eqn (8) can be transformed as follows:

$$\sigma(k+1) = \sqrt{\sum_{i=0}^{k+1}\left(\frac{i^2}{(k+1)^2}Q(i,k+1-i)\right) - \overline{x_R}^2(k+1)} =$$

$$\sqrt{\sum_{i=0}^{k+1}\left(\frac{i^2}{(k+1)^2}\left[\frac{(0.5+\varepsilon)+\alpha(i-1)}{1+\alpha\{i-1+k+1-i\}}Q(i-1,k+1-i) + \frac{(0.5-\varepsilon)+\alpha(k-i)}{1+\alpha\{i+k-i\}}Q(i,k-i)\right]\right) - (0.5+\varepsilon)^2} =$$

$$\frac{1}{(k+1)}\sqrt{\sum_{i=1}^{k+1} i^2 Q(i-1,k+1-i)\frac{(0.5+\varepsilon)+\alpha(i-1)}{1+\alpha k} + \sum_{i=0}^{k} i^2 Q(i,k-i)\frac{(0.5-\varepsilon)+\alpha(k-i)}{1+\alpha k} - (k+1)^2(0.5+\varepsilon)^2} =$$

$$\frac{1}{(k+1)}\sqrt{\sum_{i=0}^{k}(i+1)^2 Q(i,k-i)\frac{(0.5+\varepsilon)+\alpha i}{1+\alpha k} + \sum_{i=0}^{k} i^2 Q(i,k-i)\frac{(0.5-\varepsilon)+\alpha(k-i)}{1+\alpha k} - (k+1)^2(0.5+\varepsilon)^2} =$$

$$\frac{1}{(k+1)}\sqrt{\sum_{i=0}^{k} i^2 Q(i,k-i) + \sum_{i=0}^{k}(2i+1)Q(i,k-i)\frac{(0.5+\varepsilon)+\alpha i}{1+\alpha k} - (k+1)^2(0.5+\varepsilon)^2} = \qquad \text{(S39)}$$

$$\frac{1}{(k+1)}\sqrt{\sum_{i=0}^{k} i^2 Q(i,k-i) + \frac{(0.5+\varepsilon)}{1+\alpha k}\sum_{i=0}^{k}(2i+1)Q(i,k-i) + \frac{\alpha}{1+\alpha k}\sum_{i=0}^{k} i(2i+1)Q(i,k-i) - (k+1)^2(0.5+\varepsilon)^2}$$

Evaluating the expression under the square root separately gives:

$$\sum_{i=0}^{k} i^2 Q(i,k-i) + \frac{(0.5+\varepsilon)}{1+\alpha k}\sum_{i=0}^{k}(2i+1)Q(i,k-i) + \frac{\alpha}{1+\alpha k}\sum_{i=0}^{k} i(2i+1)Q(i,k-i) - (k+1)^2(0.5+\varepsilon)^2 =$$

$$= \sum_{i=0}^{k} i^2 Q(i,k-i) + 2\frac{0.5+\varepsilon}{1+\alpha k}\sum_{i=0}^{k} iQ(i,k-i) + \frac{(0.5+\varepsilon)}{1+\alpha k}\sum_{i=0}^{k} Q(i,k-i) + \frac{2\alpha}{1+\alpha k}\sum_{i=0}^{k} i^2 Q(i,k-i) +$$

$$+ \frac{\alpha}{1+\alpha k}\sum_{i=0}^{k} iQ(i,k-i) - (k+1)^2(0.5+\varepsilon)^2 = \qquad \text{(S40a)}$$

$$= k^2(0.5+\varepsilon)(0.5-\varepsilon)\frac{k^{-1}+\alpha}{1+\alpha} + k^2(0.5+\varepsilon)^2 + 2\frac{0.5+\varepsilon}{1+\alpha k}k(0.5+\varepsilon) + \frac{(0.5+\varepsilon)}{1+\alpha k} + \frac{2\alpha}{1+\alpha k}k^2(0.5+\varepsilon)(0.5-\varepsilon)\frac{k^{-1}+\alpha}{1+\alpha}$$

$$+ \frac{2\alpha}{1+\alpha k}k^2(0.5+\varepsilon)^2 + \frac{\alpha}{1+\alpha k}k(0.5+\varepsilon) - (k+1)^2(0.5+\varepsilon)^2 =$$

$$= (0.5+\varepsilon)^2\left(k^2 + k^2\,\frac{2\alpha}{1+\alpha k} + \frac{2k}{1+\alpha k} - (k+1)^2\right) + (0.5+\varepsilon)\left(\frac{1}{1+\alpha k} + \frac{k\alpha}{1+\alpha k}\right) + k^2(0.5+\varepsilon)(0.5-\varepsilon)\,\frac{k^{-1}+\alpha}{1+\alpha}\left(1+\frac{2\alpha}{1+\alpha k}\right) =$$

$$= (0.5+\varepsilon)^2\left(k^2 + \frac{2k^2\alpha + 2k}{1+\alpha k} - (k+1)^2\right) + (0.5+\varepsilon) + k(0.5+\varepsilon)(0.5-\varepsilon)\,\frac{1+\alpha k}{1+\alpha}\left(\frac{1+\alpha k + 2\alpha}{1+\alpha k}\right) =$$

(S40b)

$$= (0.5+\varepsilon)\left[(0.5+\varepsilon)[k^2 + 2k - (k+1)^2] + 1 + k(0.5-\varepsilon)\left(1+\alpha\,\frac{k+1}{1+\alpha}\right)\right] =$$

$$= (0.5+\varepsilon)\left[-(0.5+\varepsilon) + 1 + k(0.5-\varepsilon)\left(1+\alpha\,\frac{k+1}{1+\alpha}\right)\right] = (0.5+\varepsilon)\left[0.5-\varepsilon + k(0.5-\varepsilon)\left(1+\alpha\,\frac{k+1}{1+\alpha}\right)\right] =$$

$$= (0.5+\varepsilon)(0.5-\varepsilon)\left[1 + k + \frac{k\alpha(k+1)}{1+\alpha}\right] = (0.5+\varepsilon)(0.5-\varepsilon)(k+1)\,\frac{1+\alpha+\alpha k}{1+\alpha} = (0.5+\varepsilon)(0.5-\varepsilon)(k+1)\,\frac{1+\alpha(k+1)}{1+\alpha}$$

Substituting the results of eqn (S40) into eqn (S39):

$$\sigma(k+1) = \frac{1}{(k+1)}\sqrt{\sum_{i=0}^{k} i^2 Q(i,k-i) + \frac{(0.5+\varepsilon)}{1+\alpha k}\sum_{i=0}^{k}(2i+1)Q(i,k-i) + \frac{\alpha}{1+\alpha k}\sum_{i=0}^{k} i(2i+1)Q(i,k-i) - (k+1)^2(0.5+\varepsilon)^2} =$$

(S41)

$$\frac{1}{(k+1)}\sqrt{(0.5+\varepsilon)(0.5-\varepsilon)(k+1)\,\frac{1+\alpha(k+1)}{1+\alpha}} = \sqrt{(0.5+\varepsilon)(0.5-\varepsilon)\,\frac{(k+1)^{-1}+\alpha}{1+\alpha}}$$

Eqn (S41) proves that eqn (23) is true for all positive integers.

Equation (24):

In a previous work cited as reference 39 in the manuscript, it is shown that the final distribution can be obtained using the following formula:

$$f(x_r) = \lim_{(r+s)\to\infty, x_R = r/s} (r+s)Q(r,s) \tag{S42}$$

Combining eqn (S42) and eqn (21) gives:

$$f(x_r) = \lim_{(r+s)\to\infty, x_R = r/s} (r+s)Q(r,s) = \lim_{(r+s)\to\infty, x_R = r/s} (r+s)\binom{r+s}{r} \frac{\prod_{i=0}^{r-1}(0.5+\varepsilon+\alpha i)\prod_{i=0}^{s-1}(0.5-\varepsilon+\alpha i)}{\prod_{i=0}^{r+s-1}(1+\alpha i)} =$$

$$= \lim_{(r+s)\to\infty, x_R = r/s} (r+s)\frac{(r+s)!}{r!s!} \frac{\prod_{i=0}^{r-1}(0.5+\varepsilon+\alpha i)\prod_{i=0}^{s-1}(0.5-\varepsilon+\alpha i)}{\prod_{i=0}^{r+s-1}(1+\alpha i)} =$$

$$= \lim_{(r+s)\to\infty, x_R = r/s} (r+s)\frac{(r+s)}{rs} \frac{(0.5+\varepsilon)\prod_{i=1}^{r-1}(\frac{0.5+\varepsilon}{i}+\alpha)\times(0.5-\varepsilon)\prod_{i=1}^{s-1}(\frac{0.5-\varepsilon}{i}+\alpha)}{\prod_{i=1}^{r+s-1}(\frac{1}{i}+\alpha)} =$$

$$= \lim_{(r+s)\to\infty, x_R = r/s} (r+s)\frac{(r+s)}{rs} \frac{\alpha^r \frac{(0.5+\varepsilon)}{\alpha}\prod_{i=1}^{r-1}(\frac{0.5+\varepsilon}{\alpha i}+1)\times\alpha^s \frac{(0.5-\varepsilon)}{\alpha}\prod_{i=1}^{s-1}(\frac{0.5-\varepsilon}{\alpha i}+1)}{\alpha^{r+s}\frac{1}{\alpha}\prod_{i=1}^{r+s-1}(\frac{1}{i}+\alpha)} =$$

$$= \lim_{(r+s)\to\infty, x_R = r/s} \frac{(r+s)^{2-1/\alpha}}{r^{1-(0.5+\varepsilon)/\alpha}s^{1-(0.5-\varepsilon)/\alpha}} \frac{(r+s)^{1/\alpha}}{r^{(0.5+\varepsilon)/\alpha}s^{(0.5-\varepsilon)/\alpha}} \frac{\frac{(0.5+\varepsilon)}{\alpha}\prod_{i=1}^{r-1}(\frac{0.5+\varepsilon}{\alpha i}+1)\times\frac{(0.5-\varepsilon)}{\alpha}\prod_{i=1}^{s-1}(\frac{0.5-\varepsilon}{\alpha i}+1)}{\frac{1}{\alpha}\prod_{i=1}^{r+s-1}(\frac{1}{i}+\alpha)} \tag{S43}$$

The Euler limit form of the gamma function is:

$$\Gamma(z) = \lim_{k\to\infty} \frac{(k+1)^z}{z(1+z)(1+z/2)(1+z/3)\ldots(1+z/k)} \tag{S44}$$

Further transformation of eqn (S43) taking eqn (S44) into account gives

$$f(x_r) = \lim_{(r+s)\to\infty, x_R = r/s} \frac{(r+s)^{2-1/\alpha}}{r^{1-(0.5+\varepsilon)/\alpha} s^{1-(0.5-\varepsilon)/\alpha}} \frac{(r+s)^{1/\alpha}}{r^{(0.5+\varepsilon)/\alpha} s^{(0.5-\varepsilon)/\alpha}} \frac{\frac{(0.5+\varepsilon)}{\alpha}\prod_{i=1}^{r-1}(\frac{0.5+\varepsilon}{\alpha i}+1)\times\frac{(0.5-\varepsilon)}{\alpha}\prod_{i=1}^{s-1}(\frac{0.5-\varepsilon}{\alpha i}+1)}{\frac{1}{\alpha}\prod_{i=1}^{r+s-1}(\frac{1}{i}+\alpha)} =$$

$$= \lim_{(r+s)\to\infty, x_R = r/s} \left(\frac{r}{r+s}\right)^{(0.5+\varepsilon)/\alpha - 1} \left(\frac{s}{r+s}\right)^{(0.5-\varepsilon)/\alpha - 1} \frac{(r+s)^{1/\alpha}}{\frac{1}{\alpha}\prod_{i=1}^{r+s-1}(\frac{1}{i}+\alpha)} \frac{\frac{(0.5+\varepsilon)}{\alpha}\prod_{i=1}^{r-1}(\frac{0.5+\varepsilon}{\alpha i}+1)}{r^{(0.5+\varepsilon)/\alpha}} \frac{\frac{(0.5-\varepsilon)}{\alpha}\prod_{i=1}^{s-1}(\frac{0.5-\varepsilon}{\alpha i}+1)}{s^{(0.5-\varepsilon)/\alpha}} = \tag{S45}$$

$$= x_R^{(0.5+\varepsilon)/\alpha - 1}(1-x_R)^{(0.5-\varepsilon)/\alpha - 1} \frac{\Gamma\left(\frac{1}{\alpha}\right)}{\Gamma\left(\frac{0.5+\varepsilon}{\alpha}\right)\Gamma\left(\frac{0.5-\varepsilon}{\alpha}\right)}$$

The beginning and the end of eqn (S45) gives eqn (24).

Equation (25):

Eqn (S5) (which appears under the proof of eqn 7) will be used as a starting point. Variable *s* will be considered as a function of variable *r*. The lower two equations in eqn (S5) and a differentiation rule similar to the one given in eqn (S9) gives the following ordinary differential equation:

$$\frac{ds}{dr} = \frac{0.5 - \varepsilon + \alpha s^{\xi}(r)}{0.5 + \varepsilon + \alpha r^{\xi}} \qquad \text{(S46)}$$

The initial conditions are $r = 0$ and $s = 0$. First of all, note that the derivative is always positive, therefore $s(r)$ is a monotonic increasing function.
The proof presented here will be quite long and somewhat complicated. To help the understanding, the general strategy is outlined as follows:

Part 1: It will be shown that the following upper limit applies to function $s(r)$ defined by differential equation (S46):

$$\frac{s(r)}{r} < \frac{0.5 - \varepsilon}{0.5 + \varepsilon} \qquad \text{for any } r > 0 \qquad \text{(S47)}$$

Part 2: It will be shown that exactly on of the following statements is true:

2.1. Function $s(r)$ is limited and there exits a real number (Z) for which

$$\lim_{r \to \infty} s(r) \le Z \qquad \text{(S48)}$$

2.2. A suitable function $\Sigma(r)$ and a real number r_d can be defined for which

$$\Sigma(r) > s(r) \qquad \text{for any} \quad r > r_d \qquad \text{(S49)}$$

Part 3: It will be shown that from both statement 2a and 2b it follows that

$$\lim_{r \to \infty} \frac{s(r)}{r} = 0 \qquad \text{(S50)}$$

Part 4: It will be shown that eqn (25) follows from eqn (S50).

Part 1:

1.1. Eqn (S46) and the definition of the first derivative of a function gives:

$$\frac{ds}{dr}(r = 0) = \frac{0.5 - \varepsilon}{0.5 + \varepsilon} = \lim_{r \to 0} \frac{s(r) - 0}{r - 0} = \lim_{r \to 0} \frac{s(r)}{r} \qquad \text{(S51)}$$

First, number X is defined as:

$$X = \sqrt[\xi]{\frac{0.5-\varepsilon}{0.5+\varepsilon}} - \frac{0.5-\varepsilon}{0.5+\varepsilon} \tag{S52}$$

$X > 0$ because

$$\xi > 1 \qquad \text{and} \qquad 1 > \frac{0.5-\varepsilon}{0.5+\varepsilon}. \tag{S53}$$

Eqn (S51) states that function $s(r)/r$ has a limit at $r = 0$, therefore a $Y > 0$ number exists so that

$$\left|\frac{s(r)}{r} - \frac{0.5-\varepsilon}{0.5+\varepsilon}\right| < X \qquad \text{for any } 0 < r < Y \tag{S54}$$

1.2. An indirect method will be used to prove that for any $0 < r < Y$,

$$\frac{s(r)}{r} < \frac{0.5-\varepsilon}{0.5+\varepsilon} \qquad \text{for any } 0 < r < Y \tag{S55}$$

Assume that there exists an r^*, for which $0 < r^* < Y$ and

$$\frac{s(r^*)}{r^*} \geq \frac{0.5-\varepsilon}{0.5+\varepsilon} \qquad \Rightarrow \qquad s(r^*) \geq \frac{0.5-\varepsilon}{0.5+\varepsilon} r^* \tag{S56}$$

Next, Cauchy's mean-value theorem is used with the two functions $f = s(r)$ and $g(r) = r$ (http://mathworld.wolfram.com/CauchysMean-ValueTheorem.html) to show that there exists at least one r_a, for which $0 < r_a < r^* < Y$ and

$$\frac{s(r^*) - 0}{r^* - 0} = \frac{s(r^*)}{r^*} = \frac{ds}{dr}(r_a) \tag{S57}$$

Combining eqn (S57) and (S56) gives

$$\frac{ds}{dr}(r_a) \geq \frac{0.5-\varepsilon}{0.5+\varepsilon} \tag{S58}$$

From eqn (S46) it follows that

$$\frac{ds}{dr}(r_a) = \frac{0.5 - \varepsilon + \alpha s^{\xi}(r_a)}{0.5 + \varepsilon + \alpha r_a^{\ \xi}} \tag{S59}$$

Combining eqn (S59) and eqn (S58) gives

$$\frac{0.5-\varepsilon}{0.5+\varepsilon} \le \frac{0.5-\varepsilon+\alpha s^{\xi}(r_{\mathrm{a}})}{0.5+\varepsilon+\alpha r_{\mathrm{a}}^{\ \xi}} \tag{S60}$$

After rearrangement, one obtains:

$$\frac{r_{\mathrm{a}}^{\ \xi}}{0.5+\varepsilon} \le \frac{s^{\xi}(r_{\mathrm{a}})}{0.5-\varepsilon} \qquad \Rightarrow \qquad \sqrt[\xi]{\frac{0.5-\varepsilon}{0.5+\varepsilon}} \le \frac{s(r_{\mathrm{a}})}{r_{\mathrm{a}}} \tag{S61}$$

Subtracting the same number from both sides of eqn (S61) and substituting eqn (S52) gives:

$$X = \sqrt[\xi]{\frac{0.5-\varepsilon}{0.5+\varepsilon}} - \frac{0.5-\varepsilon}{0.5+\varepsilon} \le \frac{s(r_{\mathrm{a}})}{r_{\mathrm{a}}} - \frac{0.5-\varepsilon}{0.5+\varepsilon} = \left| \frac{s(r_{\mathrm{a}})}{r_{\mathrm{a}}} - \frac{0.5-\varepsilon}{0.5+\varepsilon} \right| \tag{S62}$$

However, eqn (S62) contradicts eqn (S54). Eqn S(55) must be true then.

1.3. Now, eqn (S47) can be proved with an indirect method.
Eqn (S55) shows that eqn (47) is true for any $0 < r < \mathrm{Y}$. Assume that there exists $r \ge Y$ for which

$$s(r) \ge \frac{0.5-\varepsilon}{0.5+\varepsilon} r \tag{S63}$$

Function $s(r)$ is continuous, therefore certain r values must exist at which the equation holds in eqn (S63). Let r_b the smallest such value. Consequently, this r_b satisfies the following conditions:

$$s(r_b) = \frac{0.5-\varepsilon}{0.5+\varepsilon} r_b \qquad \text{and} \qquad \frac{s(r)}{r} < \frac{0.5-\varepsilon}{0.5+\varepsilon} \quad \text{for any } r < r_b \tag{S64}$$

Because of Cauchy's mean-value theorem, there exists at least one r_{c}, for which $0 < r_{\mathrm{c}} < r_{\mathrm{b}}$ and

$$\frac{s(r_b)-0}{r_b-0} = \frac{s(r_b)}{r_b} = \frac{ds}{dr}(r_{\mathrm{c}}) \tag{S65}$$

Combining eqn (S65) and eqn (S64) gives

$$\frac{ds}{dr}(r_{\mathrm{c}}) = \frac{0.5-\varepsilon}{0.5+\varepsilon} \tag{S66}$$

From differential equation (S46) one obtains:

$$\frac{ds}{dr}(r_{\mathrm{c}}) = \frac{0.5-\varepsilon+\alpha s^{\xi}(r_{\mathrm{c}})}{0.5+\varepsilon+\alpha r_{\mathrm{c}}^{\ \xi}} \tag{S67}$$

Combining eqn (S67) and eqn (S66) gives

$$\frac{0.5-\varepsilon}{0.5+\varepsilon}=\frac{0.5-\varepsilon+\alpha s^{\xi}(r_{\mathrm{c}})}{0.5+\varepsilon+\alpha r_{\mathrm{c}}{}^{\xi}} \tag{S68}$$

After rearrangement, the following equation is obtained:

$$\frac{r_{\mathrm{c}}{}^{\xi}}{0.5+\varepsilon}=\frac{s^{\xi}(r_{\mathrm{c}})}{0.5-\varepsilon} \quad \Rightarrow \quad \frac{s(r_{\mathrm{c}})}{r_{\mathrm{c}}}=\sqrt[\xi]{\frac{0.5-\varepsilon}{0.5+\varepsilon}}>\frac{0.5-\varepsilon}{0.5+\varepsilon} \tag{S69}$$

Eqn (S69) contradicts the second condition in eqn (S64). Eqn (S44) must be true then.

Part 2:
Define r_d as the value for which

$$s(r_d) = \sqrt[\xi]{\frac{0.5-\varepsilon}{\alpha\left(\frac{0.5+\varepsilon}{0.5-\varepsilon}\right)^{(\xi-1)/2} - \alpha}} = Z \qquad \text{(S70)}$$

2.1. Function $s(r)$ is monotonic and increasing. If there is no r_d which satisfies eqn (S70), then function $s(r)$ is limited and

$$\lim_{r\to\infty} s(r) \le \sqrt[\xi]{\frac{0.5-\varepsilon}{\alpha\left(\frac{0.5+\varepsilon}{0.5-\varepsilon}\right)^{(\xi-1)/2} - \alpha}} \qquad \text{(S71)}$$

Eqn (S48) follows from eqn (S71) and eqn (S70).

2.2. If a suitable r_d exists in eqn (S70), the fact that $s(r)$ is a monotonic increasing function guarantees that

$$s(r) \ge \sqrt[\xi]{\frac{0.5-\varepsilon}{\alpha\left(\frac{0.5+\varepsilon}{0.5-\varepsilon}\right)^{(\xi-1)/2} - \alpha}} \qquad \text{for any } r \ge r_d \qquad \text{(S72)}$$

2.2.1. First it will be proved that

$$\left(\frac{s(r)}{r}\right)^{(\xi+1)/2} > \frac{ds}{dr} \qquad \text{for any } r \ge r_d \qquad \text{(S73)}$$

Rearranging eqn (S72) gives:

$$\alpha\left(\frac{0.5+\varepsilon}{0.5-\varepsilon}\right)^{(\xi-1)/2} s^{\xi}(r) r^{(\xi+1)/2} - \alpha s^{\xi}(r) r^{(\xi+1)/2} \ge (0.5-\varepsilon) r^{(\xi+1)/2} \qquad \text{(S74)}$$

Eqn (S47) can be rearranged into the following form:

$$s^{(\xi-1)/2}(r) < \left(\frac{0.5-\varepsilon}{0.5+\varepsilon}\right)^{(\xi-1)/2} r^{(\xi-1)/2} \qquad \text{(S75)}$$

Eqn (S74) and eqn (S75) can be combined to give the following formula:

$$\alpha s^{(\xi+1)/2}(r) r^{\xi} > \alpha\left(\frac{0.5-\varepsilon}{0.5+\varepsilon}\right)^{(\xi-1)/2} s^{\xi}(r) r^{(\xi+1)/2} \qquad \text{(S76)}$$

It is evident that

$$0 < (0.5+\varepsilon)s^{(\xi+1)/2}(r) \tag{S77}$$

Combining eqn (S77), eqn (S76) and (S74) gives:

$$\alpha s^{(\xi+1)/2}(r)r^{\xi} - \alpha s^{\xi}(r)r^{(\xi+1)/2} + (0.5+\varepsilon)s^{(\xi+1)/2}(r) - (0.5-\varepsilon)r^{(\xi+1)/2} > 0 \tag{S78}$$

Rearranging eqn (S78) yields:

$$\frac{s^{(\xi+1)/2}(r)}{r^{(\xi+1)/2}} > \frac{0.5-\varepsilon+\alpha s^{\xi}(r)}{0.5+\varepsilon+\alpha r^{\xi}} \tag{S79}$$

Combining eqn (S79) and eqn (S46) gives eqn (S73).

2.2.2. Consider function $\Sigma(r)$ defined as:

$$\Sigma(r) = \frac{r}{\sqrt[(\xi-1)/2]{1+Cr^{(\xi-1)/2}}} = (C+r^{(1-\xi)/2})^{-2/(\xi-1)} \tag{S80}$$

where

$$C = s^{(1-\xi)/2}(r_{\mathrm{d}}) - r_{\mathrm{d}}^{(1-\xi)/2} \tag{S81}$$

Substituting eqn (S81) into eqn (S80) show that

$$\Sigma(r_{\mathrm{d}}) = s(r_{\mathrm{d}}) \tag{S82}$$

Differentiating $\Sigma(r)$ gives

$$\begin{aligned}\frac{d\Sigma}{dr} &= (C+r^{(1-\xi)/2})^{-2/(\xi-1)} = \frac{-2}{\xi-1}(C+r^{(1-\xi)/2})^{-2/(\xi-1)-1}\frac{1-\xi}{2}r^{(1-\xi)/2-1} \\ &= (C+r^{(1-\xi)/2})^{-(\xi+1)/(\xi-1)}r^{-(\xi+1)/2} = \left(\frac{\Sigma(r)}{r}\right)^{(\xi+1)/2}\end{aligned} \tag{S83}$$

Eqn (S73) and eqn (S83) can be combined to give the following:

$$\frac{ds}{dr}(r_{\mathrm{d}}) < \left(\frac{s(r_{\mathrm{d}})}{r}\right)^{(\xi+1)/2} = \left(\frac{\Sigma(r_{\mathrm{d}})}{r}\right)^{(\xi+1)/2} = \frac{d\Sigma}{dr}(r_{\mathrm{d}}) \tag{S84}$$

Consequently, there exists a number W > *0* so that

$$\Sigma(r) > s(r) \qquad \text{for any} \quad r_{\mathrm{d}} < r < r_{\mathrm{d}} + W \tag{S85}$$

2.2.3. Eqn (S49) will be proved by an indirect method. Let's assume that eqn (S49) is not true so there are $r > r_{\mathrm{d}}$ values for which

$$\Sigma(r) \le s(r) \tag{S86}$$

Function $s(r)$ is continuous, therefore a certain r values must exist at which the equation holds in eqn (S86). Denote the smallest such value r_e.

$$s(r_{\mathrm{e}}) = \Sigma(r_{\mathrm{e}}) \tag{S87}$$

Eqn (S85) shows that $r_e \ge r_{\mathrm{d}} + W$. r_e is the smallest, so for any $r_{\mathrm{d}} < r < r_e$

$$s(r) < \Sigma(r) \qquad \text{for any } r_{\mathrm{d}} < r < r_{\mathrm{e}} \tag{S88}$$

Eqn (S88), eqn S(83) and eqn (S73) can be combined to yield the following:

$$\frac{ds}{dr}(r) < \left(\frac{s(r)}{r}\right)^{(\xi+1)/2} < \left(\frac{\Sigma(r)}{r}\right)^{(\xi+1)/2} = \frac{d\Sigma}{dr}(r) \qquad \text{for any } r_{\mathrm{d}} < r < r_{\mathrm{e}} \tag{S89}$$

Because of Cauchy's mean-value theorem there exists at least one r_{f}, for which $r_{\mathrm{d}} < r_{\mathrm{f}} < r_{\mathrm{e}}$

$$\frac{s(r_e) - s(r_d)}{\Sigma(r_e) - \Sigma(r_d)} = 1 = \frac{\frac{ds}{dr}(r_{\mathrm{f}})}{\frac{d\Sigma}{dr}(r_{\mathrm{f}})} \qquad \Rightarrow \qquad \frac{ds}{dr}(r_{\mathrm{f}}) = \frac{d\Sigma}{dr}(r_{\mathrm{f}}) \tag{S90}$$

This equation contradicts eqn (S89). Eqn (S49) must be true then.

Part 3:

For case 2.1, eqn (S71) can be used to prove that eqn (S50) is true.

$$\lim_{r\to\infty} \frac{s(r)}{r} = \frac{\lim_{r\to\infty} s(r)}{\lim_{r\to\infty} r} \le \frac{\sqrt[\xi]{\dfrac{0.5-\varepsilon}{\alpha\left(\dfrac{0.5+\varepsilon}{0.5-\varepsilon}\right)^{(\xi-1)/2} - \alpha}}}{\infty} = 0 \tag{S91}$$

For case 2.2, eqn (S49), can be used to prove that eqn (S50) is true.

$$\lim_{r\to\infty}\frac{s(r)}{r} \le \lim_{r\to\infty}\frac{\Sigma(r)}{r} = \lim_{r\to\infty}\frac{\dfrac{r}{\sqrt[(\xi-1)/2]{1+Cr^{(\xi-1)/2}}}}{r} = \frac{1}{\lim\limits_{r\to\infty}\sqrt[(\xi-1)/2]{1+Cr^{(\xi-1)/2}}} = \frac{1}{\infty} = 0 \qquad \text{(S92)}$$

Part 4

Eqn (S50) can be used to prove the following:

$$\lim_{b\to\infty} ee = \lim_{r\to\infty} ee = \lim_{r\to\infty} \frac{r}{r+s(r)} = \lim_{r\to\infty} \frac{1}{1+\frac{s(r)}{r}} = \frac{1}{1+\lim\limits_{r\to\infty}\frac{s(r)}{r}} = \frac{1}{1+0} = 1 \qquad \text{(S93)}$$

The beginning and end of eqn (S93) yields eqn (25).

Further notes:

For integer values of ξ, the differential equation in eqn (S46) can be solved analytically. Separation of the variables and integration gives:

$$\int \frac{ds}{0.5-\varepsilon+\alpha s^{\xi}(r)} = \int \frac{dr}{0.5+\varepsilon+\alpha r^{\xi}} \qquad \text{(S94)}$$

For $\xi = 2$, the implicit solution is (also taking the initial conditions, $r = 0$ and $s = 0$, into account):

$$\mathrm{arctg}\left(r\sqrt{\frac{\alpha}{0.5+\varepsilon}}\right) = \sqrt{\frac{0.5+\varepsilon}{0.5-\varepsilon}}\,\mathrm{arctg}\left(s\sqrt{\frac{\alpha}{0.5-\varepsilon}}\right) \qquad \text{(S95)}$$

The explicit solution is

$$s = \sqrt{\frac{0.5-\varepsilon}{\alpha}}\,\mathrm{tg}\left[\sqrt{\frac{0.5-\varepsilon}{0.5+\varepsilon}}\,\mathrm{arctg}\left(r\sqrt{\frac{\alpha}{0.5+\varepsilon}}\right)\right] \qquad \text{(S96)}$$

More complicated implicit solutions can be derived for $\xi = 3$.

Equation (26):

First, a limiting formula for the central binomial coefficient will be proved. The following inequity will be used a starting point (http://mathworld.wolfram.com/StirlingsApproximation.html):

$$\sqrt{2\pi}n^{n+0.5}e^{-n+1/(12n+1)} < n! < \sqrt{2\pi}n^{n+0.5}e^{-n+1/(12n)} \quad \text{(S97)}$$

Squaring the first part of eqn (S97) gives:

$$(\sqrt{2\pi}n^{n+0.5}e^{-n+1/(12n+1)})^2 < n!n! \quad \text{(S98)}$$

Applying the second part of eqn (S97) for 2*n* gives:

$$(2n)! < \sqrt{2\pi}(2n)^{2n+0.5}e^{-2n+1/(24n)} \quad \text{(S99)}$$

Dividing eqn (S99) with eqn (S98)

$$\frac{(2n)!}{n!n!} < \frac{\sqrt{2\pi}(2n)^{2n+0.5}e^{-2n+1/(24n)}}{2\pi n^{2n+1}e^{-2n+2/(12n+1)}} \quad \text{(S100)}$$

Rearranging eqn (S100) yields:

$$\binom{2n}{n} < \frac{2^{2n}}{\sqrt{n\pi}}e^{1/(24n)-2/(12n+1)} < \frac{2^{2n}}{\sqrt{n\pi}} \quad \text{(S101)}$$

Next, a limiting formula for $Q(n,n)$ will be proved. The concept of paths as used in the proof of eqn(12) and (13) will be used here as well. State (n,n) can be formed in Ξ different paths where

$$\Xi = \binom{2n}{n} \quad \text{(S102)}$$

One path is represented by a (2*n*+1)-membered series *m*, where m_i gives the number of B_R steps after step *i*. Obviously, $m_0 = 0$, $m_{2n} = n$ and $m_i \le m_{i+1}$. The probability of one path is given by

$$P_{m_0m_1m_2\cdots m_{2n}} = \prod_{i=0}^{2n-1}\frac{\aleph}{1+\alpha m_i^{\xi}+\alpha(i-m_i)^{\xi}} \quad \text{(S103)}$$

where

$$\begin{aligned} \aleph &= (0.5+\varepsilon+\alpha m_i^{\xi}) \quad \text{if} \quad m_{i+1} > m_i \\ \aleph &= (0.5-\varepsilon+\alpha(i-m_i)^{\xi} \quad \text{if} \quad m_{i+1} = m_i \end{aligned} \quad \text{(S104)}$$

Out of 2*n* overall steps, there are *n* R steps and *n* S steps. Therefore

$$P_{m_0m_1m_2\cdots m_{2n}} = \prod_{i=0}^{2n-1}\frac{1}{1+\alpha m_i^{\xi}+\alpha(i-m_i)^{\xi}}\prod_{i=0}^{n-1}(0.5+\varepsilon+\alpha m_i^{\xi})\prod_{i=0}^{n-1}[0.5-\varepsilon+\alpha(i-m_i)^{\xi}] \quad \text{(S105)}$$

The definition of m_i values ensures that

$$1+\alpha m_i^{\ \xi}+\alpha(i-m_i)^{\xi}<1+\alpha m_{i+1}^{\ \xi}+\alpha(i-m_{i+1})^{\xi} \quad \text{(S106)}$$

Rearranging eqn (S106) yields:

$$\frac{1}{1+\alpha m_{i+1}^{\ \xi}+\alpha(i-m_{i+1})^{\xi}}<\frac{1}{1+\alpha m_i^{\ \xi}+\alpha(i-m_i)^{\xi}} \quad \text{(S107)}$$

Combining eqn (S105) and eqn (S107) gives:

$$P_{m_0m_1m_2\cdots m_{2n}}<\prod_{i=0}^{n-1}\frac{1}{[1+\alpha m_i^{\ \xi}+\alpha(i-m_i)^{\xi}]^2}\prod_{i=0}^{n-1}(0.5+\varepsilon+\alpha m_i^{\ \xi})\prod_{i=0}^{n-1}[0.5-\varepsilon+\alpha(i-m_i)^{\xi}] \quad \text{(S108)}$$

Rearranging (S108) yields:

$$P_{m_0m_1m_2\cdots m_{2n}}<\prod_{i=0}^{n-1}\frac{(0.5+\varepsilon+\alpha m_i^{\ \xi})[0.5-\varepsilon+\alpha(i-m_i)^{\xi}]}{[1+\alpha m_i^{\ \xi}+\alpha(i-m_i)^{\xi}]^2} \quad \text{(S109)}$$

The inequity between the geometric mean and arithmetic mean of two numbers gives:

$$\sqrt{(0.5+\varepsilon+\alpha m_i^{\ \xi})[0.5-\varepsilon+\alpha(i-m_i)^{\xi}]}\leq\frac{0.5+\varepsilon+\alpha m_i^{\ \xi}+0.5-\varepsilon+\alpha(i-m_i)^{\xi}}{2} \quad \text{(S110)}$$

After squaring and rearranging eqn (S110):

$$\frac{(0.5+\varepsilon+\alpha m_i^{\ \xi})[0.5-\varepsilon+\alpha(i-m_i)^{\xi}]}{[1+\alpha m_i^{\ \xi}+\alpha(i-m_i)^{\xi}]^2}<\frac{1}{4} \quad \text{(S111)}$$

Combining eqn (S108) and eqn (S111):

$$P_{m_0m_1m_2\cdots m_{2n}}<\prod_{i=0}^{n-1}\frac{(0.5+\varepsilon+\alpha m_i^{\ \xi})[0.5-\varepsilon+\alpha(i-m_i)^{\xi}]}{[1+\alpha m_i^{\ \xi}+\alpha(i-m_i)^{\xi}]^2}\leq\prod_{i=0}^{n-1}\frac{1}{4}=\frac{1}{2^{2n}} \quad \text{(S112)}$$

$Q(n,n)$ can be obtained as the sum of all path probabilities:

$$Q(n,n)=\sum_{\text{all }\Xi\text{ paths}}P_{m_0m_1m_2\cdots m_{2n+1}}<\sum_{\text{all }\Theta\text{ paths}}\frac{1}{2^{2\text{n}}}=\binom{2n}{n}\frac{1}{2^{2\text{n}}} \quad \text{(S113)}$$

Combining eqn (S112) and (S101) gives:

$$Q(n,n) < \binom{2n}{n}\left(\frac{1}{2}\right)^{2n} < \frac{2^{2n}}{\sqrt{n\pi}}\left(\frac{1}{2}\right)^{2n} = \frac{1}{\sqrt{n\pi}} \qquad \text{(S114)}$$

The non-defining part of eqn (12) for $R(2k+1)$ is:

$$R(2k+1) = 2\varepsilon\sum_{i=0}^{k}\frac{Q(i,i)}{1+2\alpha i^{\xi}} \qquad \text{(S115)}$$

Combining eqn (S115) and eqn (s114):

$$R(2k+1) = 2\varepsilon\sum_{i=0}^{k}\frac{Q(i,i)}{1+2\alpha i^{\xi}} < 2\varepsilon\sum_{i=0}^{k}\frac{1}{\sqrt{\pi i}}\frac{1}{1+2\alpha i^{\xi}} = \frac{2\varepsilon}{\sqrt{\pi}}\sum_{i=0}^{k}\frac{1}{i^{0.5}+2\alpha i^{\xi+0.5}} \qquad \text{(S116)}$$

As the function after the sum at the very end of eqn (S116) is a monotonic decreasing function, the following inequity holds:

$$\frac{1}{i^{0.5}+2\alpha i^{\xi+0.5}} < \int_{i-1}^{i}\frac{di}{i^{0.5}+2\alpha i^{\xi+0.5}} \qquad \text{(S117)}$$

Substituting eqn (S117) into eqn (S116) gives:

$$R(2k+1) < 2\varepsilon + \frac{2\varepsilon}{\sqrt{\pi}}\sum_{i=1}^{k}\frac{1}{i^{0.5}+2\alpha i^{\xi+0.5}} < 2\varepsilon + \frac{2\varepsilon}{\sqrt{\pi}}\sum_{i=1}^{k}\int_{i-1}^{i}\frac{di}{i^{0.5}+2\alpha i^{\xi+0.5}} = 2\varepsilon + \frac{2\varepsilon}{\sqrt{\pi}}\int_{0}^{k}\frac{di}{i^{0.5}+2\alpha i^{\xi+0.5}} \qquad \text{(S118)}$$

The beginning and end of eqn (S118) gives eqn (26).

Equation (27):

Based on eqn (9), it can be seen that

$$Q(b,0)=\prod_{i=0}^{b-1}\frac{0.5+\varepsilon+\alpha i^{\xi}}{1+\alpha i^{\xi}}>\prod_{i=0}^{b-1}\frac{0.5+\alpha i^{\xi}}{1+\alpha i^{\xi}} \qquad \text{(S119)}$$

In a previous work cited as reference 39 in the manuscript, the following equation is proved:

$$\lim_{b\to\infty}\left(b\prod_{i=0}^{b-1}\frac{0.5+\alpha i^{\xi}}{1+\alpha i^{\xi}}\right)=\infty \qquad \text{(S120)}$$

A combination of eqn (S119) and (S120) gives eqn (27).

Equation (28):

Dviding the two parts of eqn (9) gives:

$$\frac{Q(b,0)}{Q(0,b)}=\frac{\prod_{i=0}^{b-1}\frac{0.5+\varepsilon+\alpha i^{\xi}}{1+\alpha i^{\xi}}}{\prod_{i=0}^{b-1}\frac{0.5-\varepsilon+\alpha i^{\xi}}{1+\alpha i^{\xi}}}=\prod_{i=0}^{b-1}\frac{0.5+\varepsilon+\alpha i^{\xi}}{0.5-\varepsilon+\alpha i^{\xi}}=\prod_{i=0}^{b-1}\left(1+\frac{2\varepsilon}{0.5-\varepsilon+\alpha i^{\xi}}\right) \quad \text{(S121)}$$

Taking the natural logarithm of eqn (S121) and subsequent arithmetic transformations give:

$$\ln\left(\frac{Q(b,0)}{Q(0,b)}\right)=\ln\left[\prod_{i=0}^{b-1}\left(1+\frac{2\varepsilon}{0.5-\varepsilon+\alpha i^{\xi}}\right)\right]=\sum_{i=0}^{b-1}\ln\left(1+\frac{2\varepsilon}{0.5-\varepsilon+\alpha i^{\xi}}\right) \quad \text{(S122)}$$

The Mercator series (http://mathworld.wolfram.com/MercatorSeries.html) of natural logarithm shows that for any $x>0$

$$\ln(1+x)<x \quad \text{(S123)}$$

Using eqn (S123) in eqn (S122) yields:

$$\ln\left(\frac{Q(b,0)}{Q(0,b)}\right)<\sum_{i=0}^{b-1}\frac{2\varepsilon}{0.5-\varepsilon+\alpha i^{\xi}}=2\varepsilon\sum_{i=0}^{b-1}\frac{1}{0.5-\varepsilon+\alpha i^{\xi}} \quad \text{(S124)}$$

As the function after the sum at the very end of eqn (S124) is a monotonic decreasing function, the following inequity holds:

$$\frac{1}{0.5-\varepsilon+\alpha i^{\xi+0.5}}<\int_{i-1}^{i}\frac{di}{0.5-\varepsilon+\alpha i^{\xi}} \quad \text{(S125)}$$

Substituting eqn (S125) into eqn (S124) gives:

$$\ln\left(\frac{Q(b,0)}{Q(0,b)}\right)<\frac{2\varepsilon}{0.5-\varepsilon}+2\varepsilon\sum_{i=1}^{b-1}\frac{1}{0.5-\varepsilon+\alpha i^{\xi}}<\frac{2\varepsilon}{0.5-\varepsilon}+2\varepsilon\sum_{i=1}^{b-1}\int_{i-1}^{i}\frac{di}{0.5-\varepsilon+\alpha i^{\xi}}=$$

$$=\frac{2\varepsilon}{0.5-\varepsilon}+2\varepsilon\int_{0}^{b-1}\frac{di}{0.5-\varepsilon+\alpha i^{\xi}}<\frac{2\varepsilon}{0.5-\varepsilon}+2\varepsilon\int_{0}^{1}\frac{di}{0.5-\varepsilon}+2\varepsilon\int_{1}^{b-1}\frac{di}{\alpha i^{\xi}} \quad \text{(S126)}$$

Calculating the integrals (for $\xi>1$) indicated at the end of eqn (126) gives:

$$2\varepsilon\int_{0}^{1}\frac{di}{0.5-\varepsilon}+2\varepsilon\int_{1}^{b-1}\frac{di}{\alpha i^{\xi}}=\frac{2\varepsilon}{0.5-\varepsilon}+\frac{2\varepsilon(\xi-1)}{\alpha 1^{\xi-1}}-\frac{2\varepsilon(\xi-1)}{\alpha(b-1)^{\xi-1}}<\frac{2\varepsilon}{0.5-\varepsilon}+\frac{2\varepsilon(\xi-1)}{\alpha} \quad \text{(S127)}$$

Combining eqn (S126) and eqn (S127) gives:

$$\ln\left(\frac{Q(b,0)}{Q(0,b)}\right) < \frac{4\varepsilon}{0.5-\varepsilon} + \frac{2\varepsilon(\xi-1)}{\alpha} \tag{S128}$$

Straightforward transformation of eqn (S128) gives eqn (28).

Equation (29):

Rearranging equation (28) yields:

$$\frac{bQ(b,0)}{e^{4\varepsilon/(0.5-\varepsilon)+2(\xi-1)\varepsilon/\alpha}} < bQ(0,b) \tag{S129}$$

Equation (27) show that

$$\lim_{b\to\infty}\frac{bQ(b,0)}{e^{4\varepsilon/(0.5-\varepsilon)+2(\xi-1)\varepsilon/\alpha}} = \frac{\lim_{b\to\infty} bQ(b,0)}{e^{4\varepsilon/(0.5-\varepsilon)+2(\xi-1)\varepsilon/\alpha}} = \frac{\infty}{e^{4\varepsilon/(0.5-\varepsilon)+2(\xi-1)\varepsilon/\alpha}} = \infty \tag{S130}$$

A combination of eqn (S129) and eqn (S130) gives eqn (29).

Methods for estimating regions in Fig 2:

The boundary of the high *ee* region was calculated by direct calculation of $E(N)$ from eqn (8) and eqn (18) for low (< 1000) values of N. For larger values of N, the continuous distribution given in eqn (24) is valid and the critical value of α from the cumulative distribution function obtained by numerically integration of the distribution function.

The boundary of the *de lege* region was calculated by applying eqn (26) for $\xi = 1$ followed by numerical integration.

The boundaries of the stochastic region and the significant B_R excess region were calculated directly using eqn (23).

Methods for estimating region in Fig. 3

The boundary of the *de lege* region was calculated by applying eqn (26) for $\xi > 1$ followed by numerical integration.

The boundaries of the high *ee* region and stochastic region were estimated as follows:

– For low (< 5000) values of N, $\sigma(N)$ was directly calculated by determining each $Q(r,s)$ value with the recursive definition given in eqn (8).

– For high values of N, a mixed stochastic-deterministic approach very similar to the one used in reference 39 was used. For every value of α, a small N_0 was found for which the autocatalytic part of the rate equations was negligibly small compared to the non-catalytic part. It is known that the distribution for a system with non-catalytic reactions only is a binomial distribution. This can be approximated very well with a normal distribution for large values of N. 100 points were selected from this distribution equidistantly scattered in the cumulative distribution function. Eqn (7) was numerically integrated with the Runge-Kutta algorithm for all these 100 initial conditions. Therefore estimates for $\sigma(N)$ were obtained for $N > N_0$ values. N_0 was selected to be the smallest possible value for which the numerical integration showed

$$\frac{\sigma(1.02 \times N_0)}{\sigma(N_0)} > \sqrt{1.02}$$

Methods for estimating lines in Fig. 4.

The boundary of the *de lege* region was calculated by applying integrating eqn (26) followed by numerical integration up to 10^{46}. The high *ee* region was estimated by numerical integration of eqn (7) and finding the values of α at which $ee(N=10^{46}) = 0.9$ or $ee(N=10^{40}) = 0.9$, respectively.