The ABC model: spatial structures in systems with reflection asymmetric long range interactions

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Generalized ABC Model (Evans et al., Clincy et al.)

This is a three species system where each lattice site is occupied by either an A, B or C type particle. Let $\eta_\alpha(i) = 1(0)$ if site i is (is not) occupied by a particle of species $\alpha, \alpha = 1, 2, 3, (A, B, C)$, $i = 1, \cdots, N$. A configuration $\underline{\eta}$ of this system then consists of specifying all the $\eta_\alpha(i)$, with $\sum_{\alpha=1}^{3} \eta_\alpha(i) = 1$ and $\sum_{i=1}^{N} \eta_\alpha(i) = N_\alpha$.

We consider such a system in 1D on a closed interval with N sites (or on a ring of N sites with cyclic boundary conditions $N+1 = 1$), with nearest neighbor exchanges between a particle of species α at site i and a particle of species γ at site $i+1$, $i = 1, \cdots, N-1$ on the interval (clockwise on ring) with weakly asymmetric rates specified by parameters β and $\{v_\alpha\}$,

$$q_{\alpha\gamma} = \begin{cases} e^{-3\beta\, v_{\alpha+2}/N} \approx 1 - 3\beta v_{\alpha+2}/N & \text{for } \gamma = \alpha + 1 \\ 1 & \text{for } \gamma = \alpha + 2 \end{cases}, \qquad (1)$$

It is “easy” to see that on the **interval**, the dynamics satisfy detailed balance with respect to the **canonical** Gibbs measure $\nu_\beta(\underline{\eta})$,

$$\nu_\beta(\underline{\eta}) = \exp[-\beta E_N(\underline{\eta})]/Z$$

with a reflection asymmetric mean field type energy,

$$E_N(\underline{\eta}) = \frac{3}{N} \sum_\alpha \sum_{i,j=1}^{N} \theta(j-i)\, v_{\alpha+1} \eta_\alpha(i) \eta_{\alpha+2}(j)$$

where $\theta(k) = 0$ if $k \leq 0$ and 1 otherwise. The dynamics is ergodic for finite β. Consequently $\nu_\beta(\underline{\eta})$ is the unique stationary measure, for $\beta < \infty$, $N < \infty$.

We can, without loss of generality, set $\sum_\alpha v_\alpha = 1$. The case $v_\alpha = 1/3$ was previously solved. The more general case is equivalent to adding external fields to the system, $\xi_\alpha = v_{\alpha+2} - v_{\alpha+1}$.

Note that unlike the case of the usual symmetric mean field model whose energy is independent of the dimension or topology of the lattice, the form of $E_N(\underline{\eta})$ is specifically one-dimensional.

It is easy to check that **if and only if** $r_\alpha \equiv N_\alpha/N = v_\alpha$ (this can only happen for special $v_\alpha > 0$, for all α) then the energy $E_N(\underline{\eta})$ is also well defined on the ring, i.e. it is independent of the starting site. Thus we can (mentally) connect site N to site 1 clockwise, and "rotate" each configuration on the interval without any cost in energy. The stationary measure is then the same on the interval and on the ring, and is given by $\nu_\beta(\underline{\eta})$.

In fact the observation about the relation between the ABC dynamics and the equilibrium measure with long range interactions was first made for the ring by Evans, et al.

When the r_α are not all equal to v_α the stationary state on the ring is not an equilibrium state and is in fact largely unknown. Unlike in the equilibrium case the system will now have a steady current: $J_\alpha \neq 0$ for some (or all) α.

Setting $i = x/N$ and taking the limit $N \to \infty$ the system will be described by profiles $\{\rho_A(x), \rho_B(x), \rho_C(x)\}$ with $0 \leq x \leq 1$. These will satisfy

$$0 \leq \rho_\alpha(x) \leq 1, \qquad \sum_\alpha \rho_\alpha(x) = 1, \qquad \int_0^1 \rho_\alpha(x)\mathrm{d}x = r_\alpha.$$

Considering the equilibrium system described by the Gibbs canonical distribution ν_β on the interval the typical equilibrium macroscopic density profiles $\underline{\rho}(x) = \{\rho_\alpha(x)\}$ are the minimizers of the Helmholtz free energy per site which is given by $\mathcal{F}(\{\rho_\alpha\}) = e(\{\rho_\alpha\}) - \beta^{-1} s(\{\rho_\alpha\})$, with

$$\begin{aligned} e(\{\rho_\alpha\}) &= \int_0^1 dx \int_0^1 dy\, \theta(x-y)\, 3v_{\alpha+1}\rho_\alpha(x)\rho_{\alpha+2}(y) \\ s(\{\rho_\alpha\}) &= \int_0^1 dx\, \rho_\alpha(x) \ln(\rho_\alpha(x)). \end{aligned}$$

e and s are respectively the energy and entropy per site.

We want to determine whether there is a unique, "typical," limiting profile on the interval $[0,1]$, i.e. a unique minimizer of $\mathcal{F}$ subject to the constraints above, or not.

The variation of the free energy yields the Euler-Lagrange equations (ELE),

$$\rho_\alpha(x) = \rho_\alpha(0)\mathrm{exp}\left(3\beta\int_0^x \left(v_{\alpha+1}\rho_{\alpha-1}(y) - v_{\alpha-1}\rho_{\alpha+1}(y)\right) dy\right)$$

or in the more convenient differential form

$$\frac{d\rho_\alpha(x)}{dx} = 3\beta\rho_\alpha\left(v_{\alpha+1}\rho_{\alpha+2}(x) - v_{\alpha+2}\rho_{\alpha+1}(x)\right).$$

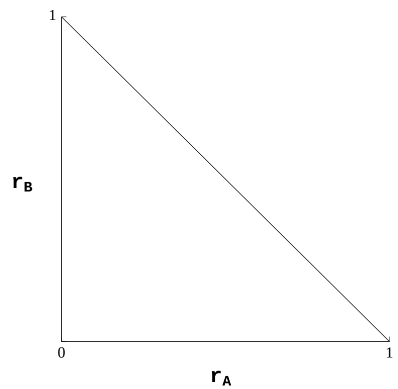
Summing over α yields $\sum_\alpha \frac{d\rho_\alpha}{dx} = 0$, consistent with $\sum_\alpha \rho_\alpha(x) = 1$.

Multiplying by v_α/ρ_α and summing over α yields another "conserved" quantity,

$$\rho_A^{v_A}(x)\rho_B^{v_B}(x)\rho_C^{v_C}(x) = K, \qquad \text{independent of x.}$$

There are thus two constants of motion (Nambu dynamics).

The solutions of the ELE correspond to the stationary points of $\mathcal{F}$ which are in the interior of the domain of permissible density profiles, *i.e.*, $\rho_\alpha(x) > 0$ for each α with $x \in [0, 1]$ as long as $r_\alpha \neq 0$.



There will always be at least one such interior solution of the ELE corresponding to the minimizer(s) of $\mathcal{F}$, at nonzero temperature, $\beta < \infty$, due to the form of the entropy terms. These ensure that the minimizer does not occur on the boundary of the triangle.

N.B. If, and only if, $r_\alpha = v_\alpha$ then $\rho_\alpha(x) = r_\alpha$ is a solution of the ELE, which may or may not be a minimizer.

Solution of the ELE for the "standard" case, $v_\alpha = 1/3$, all α

Using the constants of motion we find that each $\rho_\alpha(x)$ is a solution of

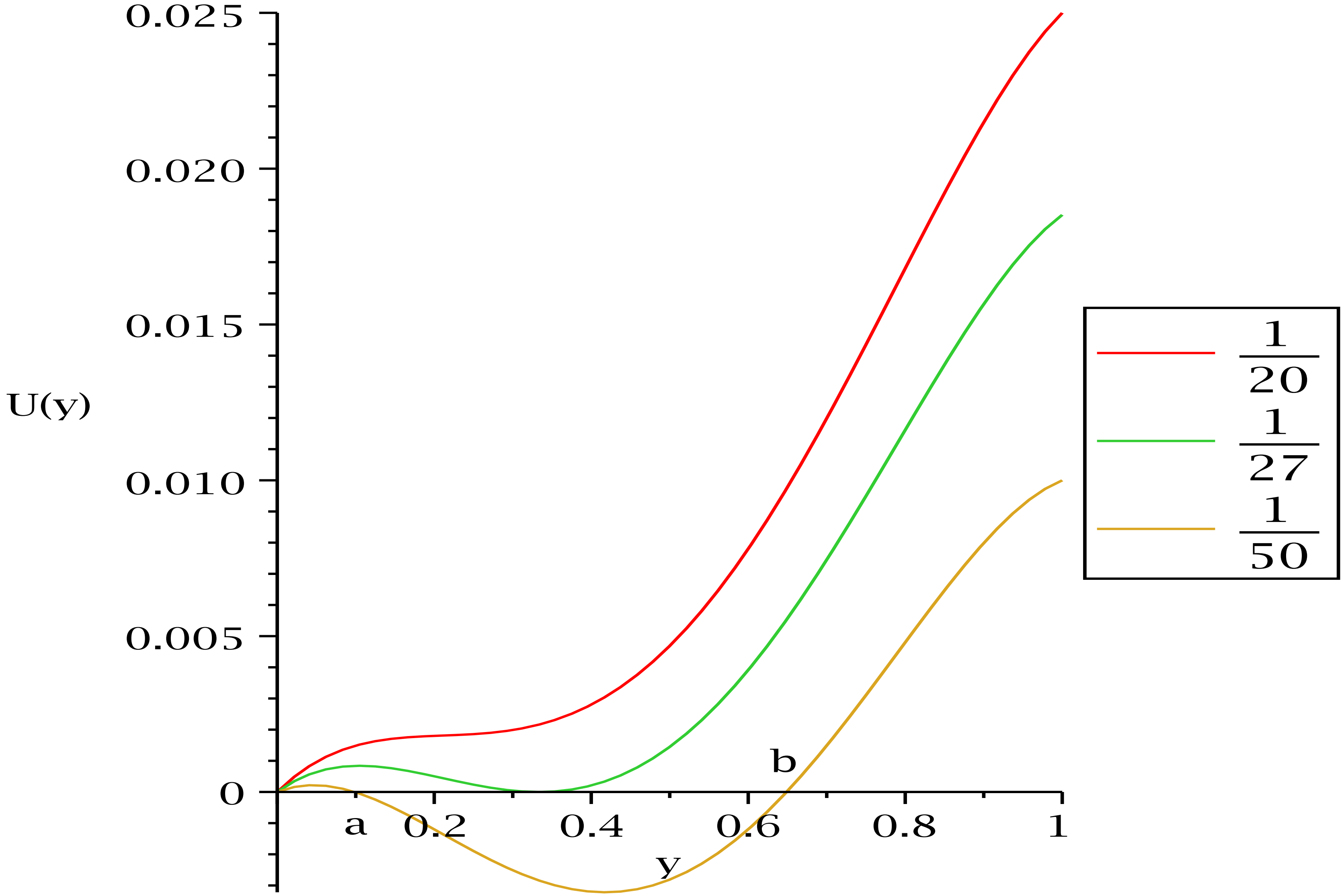
$$\rho'(x)^2 + 8\beta^2 U_K(\rho(x)) = 0; \qquad U_K(\rho) \equiv \frac{1}{2}K\rho - \frac{1}{8}\rho^2(1-\rho)^2.$$

Set $t = 2\beta x$ and let $y(t) = \rho(t/2\beta)$; then y satisfies the equation

$$\frac{1}{2}y'(t)^2 + U_K(y(t)) = 0.$$

This is the equation describing the motion of a mass 1 particle moving in a potential U_K with zero energy. For $0 < K < 1/27$, U_K has four zeros, with $U_K(y) < 0$ for $a < y < b$. See Figure. Since we are interested in solutions which satisfy $0 < \rho_\alpha(x) < 1$ we consider only the solutions $y_K(t)$ which oscillate between a and b with period τ_K.

Using these solutions (which can be expressed in terms of elliptic functions) plus some additional work we can obtain the density profiles and the phase diagram of the system.



Plots of $U_K(y)$ for $K = 1/20$, $1/27$ and $1/50$.

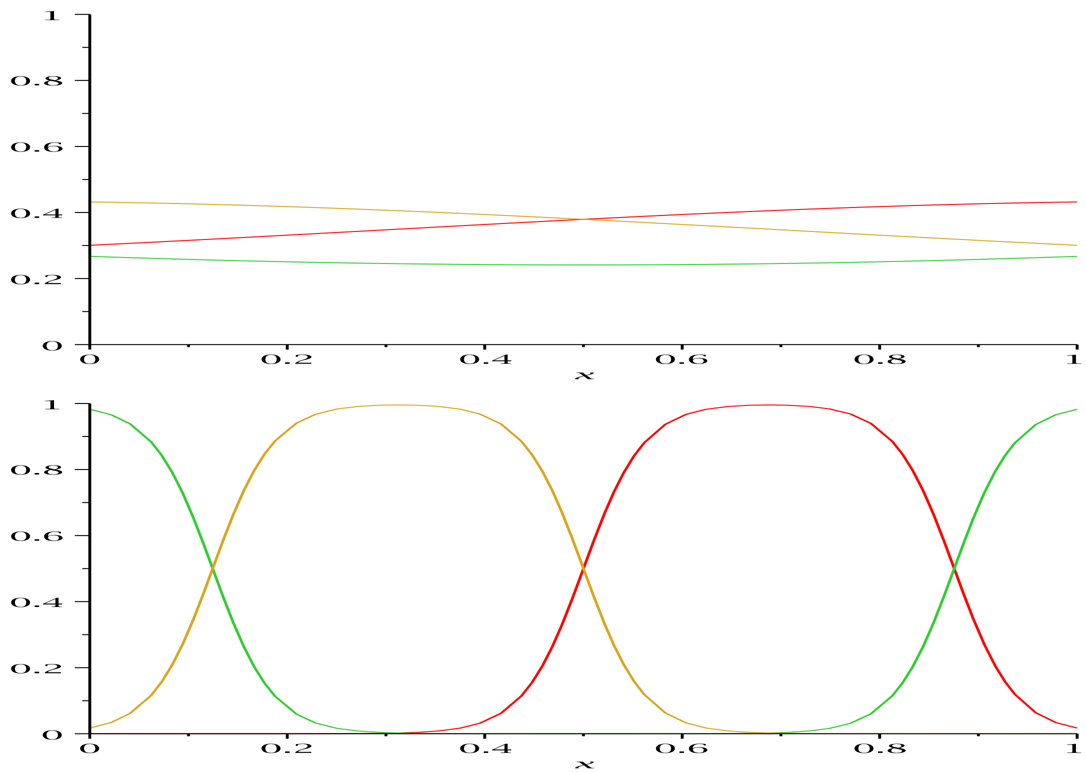
To obtain solutions $\rho_\alpha(x)$ for some K one views the curves $y_K(t)$, $t = 2\beta x$, in a window of length 2β: the different ρ_α are given by a shift of the curves by $\tau_K/3$ with the origin determined by the requirement that $\int_0^1 \rho_\alpha(x)\mathrm{d}x = r_\alpha$.

We label the solutions of the ELE by an integer which is one more than the number of full periods τ_K that fit into the window of length 2β.

A solution $\rho(x)$ of the ELE with $K < 1/27$ is of <u>type n</u>, for $n = 1, 2, \ldots,$ if $(n-1)T_K < 2\beta \leq nT_K$.

There will in general be many solutions for the ELE for a given β and $\{r_\alpha\}$. We know that <u>at least one</u> of these solutions will be the minimizer of $\mathcal{F}$.

The figure below shows the free energy minimizing profiles $\rho_\alpha(x)$ obtained from $y_K(t)$ and $y_K(t \pm T_K/3)$ for two values of β, with the same r_α's.

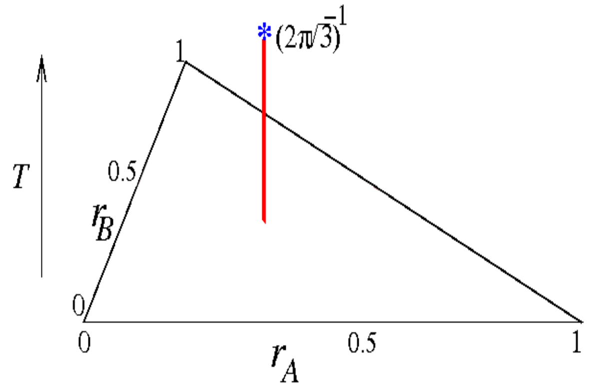


Plots of ρ_A (red), ρ_B (green), ρ_C (yellow) when $r_B = 0.25, r_A = r_C = 0.375$.
(1) $\beta = 2.898, K = 5/144$, (2) $\beta = 32.5683, K = 1/204800$.

Theorem: For $\underline{r} = (1/3, 1/3, 1/3)$ and $\beta \leq 2\pi\sqrt{3}$ there is a unique solution of the ELE and therefore ipso facto a unique minimizer. It is (as expected from Clincy et al.) $\rho_\alpha(x) = r_\alpha = 1/3$ corresponding to $K = 1/27$.

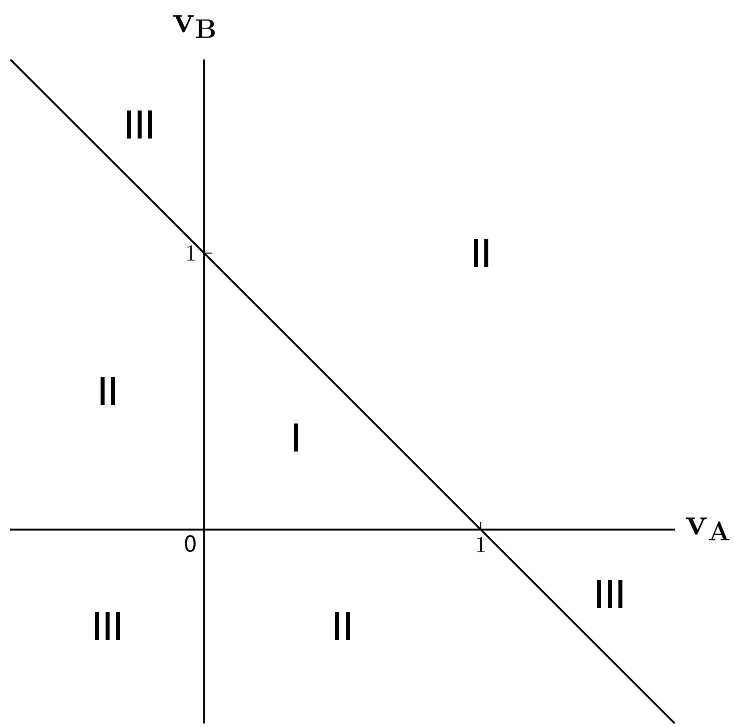
For $\underline{r} = (1/3, 1/3, 1/3)$ and $\beta > 2\pi\sqrt{3}$ all type 1 solutions with $2\beta = T_K$ and t_B any point in $[0, T_K]$ are minimizing profiles, i.e. there is a <u>continuum of minimizing solutions</u> related by a rotation. The constant solution as well as the $n > 1$ type solutions, which will exist for $\beta > 2\pi n\sqrt{3}$ are not minimizers.

For $r \neq (1/3, 1/3, 1/3)$ there is a unique minimizer for all $\beta < \infty$. It is of type 1.



Phase diagram of the standard ABC system on the interval.

Returning to the case of a more general v_α, with $\sum_\alpha v_\alpha = 1$, we divide the parameter space of the v_α into three regions.

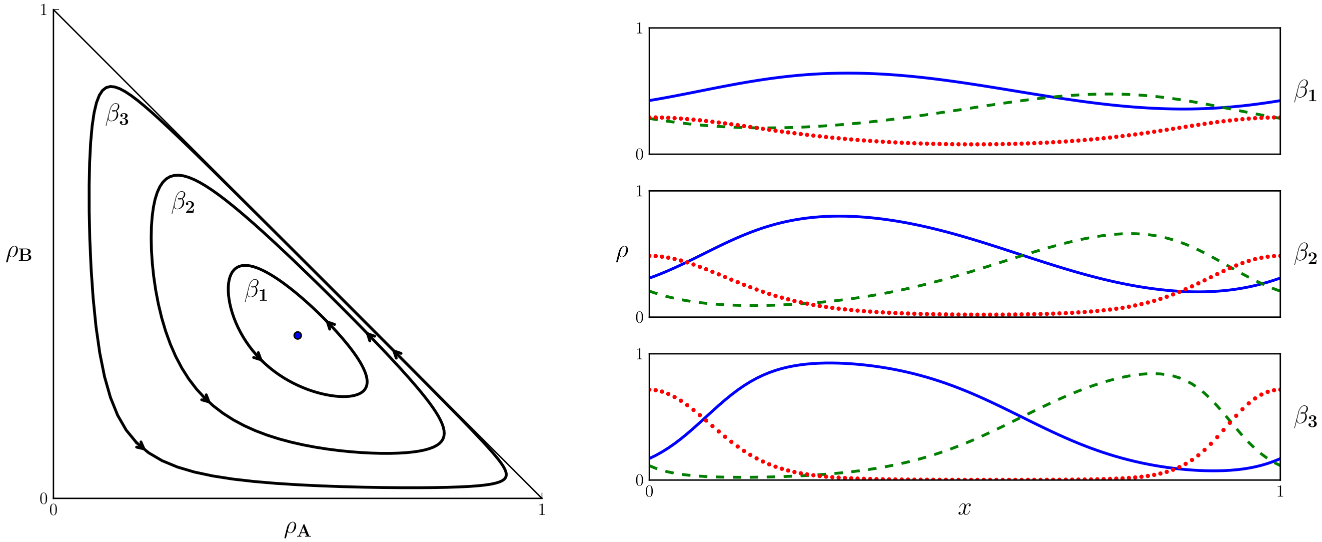


Region I: $v_\alpha > 0$ for all α,

Region II: $v_\alpha < 0$ for one value of α

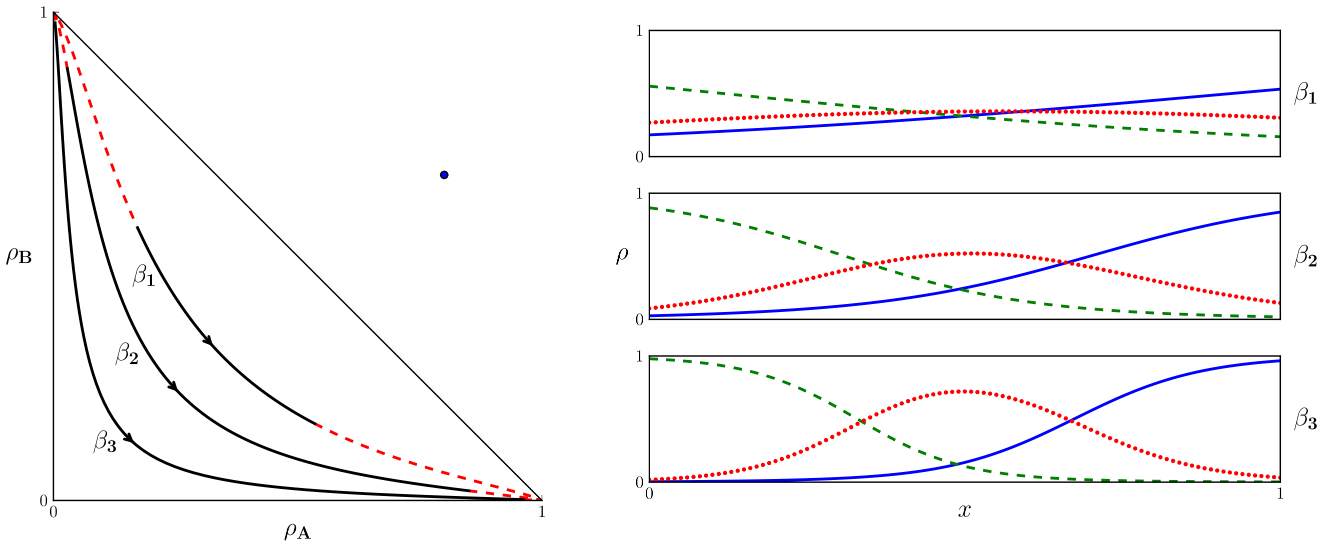
Region III: $v_\alpha < 0$ for two values of α

When the v_α lie in region I, level sets of K consist of a single point or simple closed curves surrounding that point.



Numerical solutions of the ELE and corresponding single period curves with $v_A = 1/2$, $v_B = 1/3$, $v_C = 1/6$.

When the v_α lie in regions II or III, level sets of K are open curves connecting two vertices of the triangle $\rho_A, \rho_B \geq 0$, $\rho_A + \rho_B \leq 1$.



Numerical solutions of the ELE and corresponding curves with $v_A = 4/5$, $v_B = 2/3$, $v_C = -7/15$.

Unlike the standard case $v_A = v_B = v_C = 1/3$, we cannot solve the ELE in general. However there are many similarities.

Conjecture: The phase diagram of the generalized model is qualitatively similar to the standard case. That is, (*i*) If $r_\alpha = v_\alpha$ for all α, then for $\beta \le \beta_c = \frac{2\pi}{3\sqrt{v_A v_B v_C}}$ the constant solution $\rho_\alpha(x) = v_\alpha$ minimizes $\mathcal{F}$. At β_c there is a second order phase transition, and for $\beta > \beta_c$ the minimizer is a nonconstant solution with period 1.

(*ii*) When $r_\alpha \ne v_\alpha$ for all α, there exists a unique solution of the ELE for all β.

We can prove this conjecture in several special cases.

In addition to the standard model ($v_A = v_B = v_C = 1/3$) considered previously, we are also able to prove the conjecture (by getting an explicit solution) for the case $r_\alpha = v_\alpha$, when two of the v_α are equal to 1/4 and the third is 1/2.

Part (*ii*) is proved for all β for values of the v_α lying on the boundaries between regions II and III.

We also know that the free energy is globally convex for $\beta < 4\pi/3$, so there is a unique solution for high temperatures. In particular the constant solution $\rho_\alpha = v_\alpha$ must be the minimizer at $\beta < 4\pi/3$.

The constant solution becomes linearly unstable at β_c. For $\beta > \beta_c$ a nonconstant solution with period 1 in x must be the minimizer for $r_\alpha = v_\alpha$.

Connection with Lotka-Volterra (predator-prey) equations.

Setting $t = \beta x$, solutions of the ELE in t, in the $r_\alpha = v_\alpha$ case, that have a particular value of K will have period τ_K. How does this period vary with K?

If one could show that the τ_K was a monotonically decreasing function of K, then part (*i*) of the conjecture would be proven.

Numerically, this monotonicity has been checked for many values of the v_α, and seems to hold in all cases.

In fact, the ELE for the generalized ABC model can be put in the form of the generalized Lotka-Volterra family of ODEs, which have periodic solutions:

$$\dot{x} = -y - bx^2 - cxy + by^2,$$
$$\dot{y} = x + xy.$$

The question of the monotonicity of the period for periodic solutions of this family of equations is thus directly related to our problem. It is still an open question.