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Phase transitions in autonomous reaction–diffusion systems on a one-dimensional lattice with boundaries

Amir Aghamohammadi[1] **and Mohammad Khorrami**[2]

[1] Department of Physics, Alzahra University, Tehran 19384, Iran
[2] Institute for Advanced Studies in Basic Sciences, PO Box 159, Zanjan 45195, Iran

E-mail: mohamadi@theory.ipm.ac.ir and mamwad@iasbs.ac.ir

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Abstract

The family of *autonomous* reaction–diffusion models on a one-dimensional lattice with boundaries is studied. By autonomous, it is meant that the evolution equation for n-point functions contains only n- or less than n-point functions. It is shown that these models exhibit a static and a dynamic phase transition.

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1. Introduction

Two main subjects of statistical mechanics are the study of equilibrium and non-equilibrium statistical systems. Much is known about equilibrium statistical mechanics, but the study of the non-equilibrium systems is not so well established. There are, however, many interesting problems related to the non-equilibrium behaviour of statistical systems, including the relaxation towards the stationary state. Some interesting problems in non-equilibrium systems are non-equilibrium phase transitions described by phenomenological rate equations, and the way the system relaxes to its steady state. Mean-field techniques, generally, do not give correct results for low-dimensional systems, so people are motivated to study exactly-solvable stochastic models in low dimensions. Moreover, solving one-dimensional systems should in principle be easier. Exact results for some models on a one-dimensional lattice have been obtained, for example in [1–13]. Different methods have been used to study these models, including analytical and asymptotic methods, mean-field methods and large-scale numerical methods.

Among the phenomenological models describing the relaxation of systems towards equilibrium, one can name the Glauber model and the Kawasaki model [14–19]. The combination of these two dynamics has been also considered [20–22].

In [23], an asymmetric generalization of the zero-temperature Glauber model on a lattice with boundaries was introduced. It was shown there that in the thermodynamic limit the system shows two kinds of phase transition. One of these is a static phase transition, the

other a dynamic one. The static phase transition is controlled by the reaction rates, and is a discontinuous change of the behaviour of the derivative of the stationary particle density at the end points, with respect to the reaction rates. The dynamic phase transition is controlled by the injection and extraction rates of the particles at the end points, and is a discontinuous change of the relaxation time towards the stationary configuration. Other generalizations of the Glauber model consist of, for example, alternating isotopic chains and alternating bound chains (see e.g. [24]). People have also considered phase transitions induced through boundary conditions (see, e.g. [25, 26]).

In [27], a ten-parameter family of reaction–diffusion reactions was introduced, for which the evolution equation of n-point functions contains only n- or less than n-point functions. What we do in this paper is to investigate these systems on a finite lattice with boundaries. It will be shown that the stationary behaviour of the system is effectively controlled by two parameters. On the one-dimensional boundary of this two-dimensional parameter space, there exists a phase transition (in the thermodynamic limit, when the lattice becomes infinite), which we call a static phase transition.

The relaxation time toward the stationary state of the system may depend on the injection and extraction rates at each of the boundaries. It will be shown that in the thermodynamic limit there are three regions: in one of them this time is independent of the injection and extraction rates, in the second it depends on the injection and extraction rates at one end and in the third it depends on the injection and extraction rates at the other end. This is called the dynamic phase transition.

The scheme of the paper is as follows. In section 2, autonomous reaction–diffusion systems with boundaries are introduced. In section 3, the static phase transition of these systems is investigated. Finally, in section 4, the dynamic phase transition is studied.

2. Autonomous reaction–diffusion systems with boundaries

Consider a collection of particles drifting and reacting on a one-dimensional lattice with L sites. Each site may be occupied, A, the state corresponding to which is denoted by $|1\rangle$, or empty, $\emptyset$, the state of which is denoted by $|0\rangle$. The rate of change of the state $|\alpha\beta\rangle$ to the state $|\gamma\delta\rangle$ is $H^{\gamma\delta}_{\alpha\beta}$. It is shown in [27] that the evolution equations for n-point functions are closed (involve only n- or less than n-point functions) iff the following conditions are satisfied by H:

$$\begin{aligned} &-H^{01}_{11} - H^{00}_{11} + H^{01}_{10} + H^{00}_{10} - H^{11}_{01} - H^{10}_{01} + H^{11}_{00} + H^{10}_{00} =: 0 \\ &-H^{10}_{11} - H^{00}_{11} - H^{11}_{10} - H^{01}_{10} + H^{10}_{01} + H^{00}_{01} + H^{11}_{00} + H^{01}_{00} =: 0. \end{aligned} \tag{1}$$

Defining

$$\begin{aligned} u &:= H^{10}_{01} + H^{00}_{01} \\ v &:= H^{01}_{10} + H^{00}_{10} \\ \bar{u} &:= H^{10}_{11} + H^{00}_{11} \\ \bar{v} &:= H^{01}_{11} + H^{00}_{11} \\ w &:= H^{11}_{00} + H^{10}_{00} \\ s &:= H^{11}_{00} + H^{01}_{00} \\ \bar{w} &:= H^{11}_{01} + H^{10}_{01} \\ \bar{s} &:= H^{11}_{10} + H^{01}_{10} \end{aligned} \tag{2}$$

one can write (1) as

$$\begin{aligned} u + s &= \bar{u} + \bar{s} \\ v + w &= \bar{v} + \bar{w}. \end{aligned} \tag{3}$$

At the end sites 1 and L, there are also injection and extraction rates. The injection and extraction rates at the first site are denoted by a and a', respectively. The corresponding rates at the last site are denoted by b and b'. It is then seen that

$$\begin{aligned} \langle \dot{n}_k \rangle &= -(v + w + u + s)\langle n_k \rangle + (v - \bar{v})\langle n_{k+1} \rangle + (u - \bar{u})\langle n_{k-1} \rangle + w + s \qquad 1 < k < L \\ \langle \dot{n}_1 \rangle &= -(v + w)\langle n_1 \rangle + (v - \bar{v})\langle n_2 \rangle + w + a(1 - \langle n_1 \rangle) - a'\langle n_1 \rangle \\ \langle \dot{n}_L \rangle &= -(u + s)\langle n_L \rangle + (u - \bar{u})\langle n_{L-1} \rangle + s + b(1 - \langle n_L \rangle) - b'\langle n_L \rangle \end{aligned} \tag{4}$$

where $\langle n_k \rangle$ is the probability that the kth site is occupied. Comparing this with [23], it is seen that the model considered there is a special case of this model with $\bar{u} = \bar{v} = w = s = 0$.

3. The static phase transition of the system

The steady-state solution to (4) is

$$\langle n_k \rangle = C + D_1 z_1^k + D_2 z_2^{k-L-1} \tag{5}$$

where $z_{1,2}$ satisfy

$$-(u + v + w + s) + (v - \bar{v})z_{1,2} + (u - \bar{u})z_{1,2}^{-1} = 0 \tag{6}$$

and z_2 is the root whose absolute value is greater. Let us consider this equation more carefully. Defining three new parameters p, q and r through

$$\begin{aligned} p &:= v - \bar{v} \\ q &:= u - \bar{u} \\ r &:= u + s + v + w = u + s + \bar{v} + \bar{w} = \bar{u} + \bar{s} + v + w = \bar{u} + \bar{s} + \bar{v} + \bar{w} \end{aligned} \tag{7}$$

(where (3) has been used), equation (6) is rewritten as

$$p\, z^2 - r\, z + q = 0. \tag{8}$$

Using (7) and the fact that the rates are non-negative, it is seen that

$$r \geqslant |p|, |q|, |p + q|, |p - q|. \tag{9}$$

The boundaries of the physical parameter space are thus

$$r = |p + q| \qquad \text{and} \qquad r = |p - q|. \tag{10}$$

For $r = p + q$, it is seen that $\bar{u} = \bar{v} = s = w = 0$, which means that AA and $\emptyset\emptyset$ do not change. So, there are two equilibrium states on an infinite lattice without injection or extraction; either all of the sites are occupied, or all of them are unoccupied. For $p + q = -r$, one has $u = v = \bar{s} = \bar{w} = 0$, which means that $A\emptyset$ and $\emptyset A$ do not change. So, there are two equilibrium states on an infinite lattice without injection or extraction: $\cdots A\emptyset A\emptyset \cdots$ and $\cdots \emptyset A\emptyset A \cdots$.

For $r = q - p$, one has $\bar{u} = v = s = \bar{w} = 0$. The only nonzero rates are then $H_{01}^{00} = H_{10}^{11}$ and $H_{11}^{01} = H_{00}^{10}$. As all of the configurations can be converted to each other through the reactions, the equilibrium state of the infinite lattice without injection or extraction is unique. It is not difficult to see that for the special case where these four nonzero rates are equal, this state is $\cdots (\frac{1}{2})(|0\rangle + |1\rangle) \otimes (\frac{1}{2})(|0\rangle + |1\rangle) \otimes \cdots$. For $r = p - q$, one has $u = \bar{v} = \bar{s} = w = 0$. The only nonzero terms are then $H_{10}^{00} = H_{00}^{11}$ and $H_{11}^{10} = H_{00}^{01}$. This is the same as the case $r = q - p$, with left and right sides interchanged.

Also, if $r = 0$, then $u = \bar{u} = v = \bar{v} = w = s = 0$, so $\langle \dot{n}_k \rangle = 0$, $1 < k < L$. Neglecting this trivial case, it is seen that r is positive and there are two parameters determining the behaviour of the roots of (8):

$$P(z) := p' z^2 - z + q' = 0 \tag{11}$$

where

$$\begin{aligned} p' &:= p/r \\ q' &:= q/r. \end{aligned} \tag{12}$$

Noting that $P(1) < 0$ and $P(-1) > 0$ for $r > |p + q|$, it is seen that both of the roots of (11) are real: one of them is between 1 and -1; the other is out of this interval. So, $|z_1| < 1 < |z_2|$ for $r > |p + q|$. In the thermodynamic limit $L \to \infty$,

$$\begin{aligned} \langle n_k \rangle &\approx C + D_1 z_1^k && k \ll L \\ \langle n_k \rangle &\approx C + D_2 z_2^{k-L-1} && L - k \ll L. \end{aligned} \tag{13}$$

z_1, z_2, C, D_1 and D_2 are continuous functions of the rates. So the behaviour of $\langle n_k \rangle$ near the ends of the lattice varies continuously with rates, and there is no phase transition.

If $r = p + q$, one of the roots of (11) is unity; the other is $q'/p' = q/p$. If $q > p$, then $z_1 = 1$ and $\langle n_k \rangle$ is flat for $k \ll L$. This is independent of p and q. However, if $q < p$, then $z_2 = 1$ and the slope of $\langle n_k \rangle$ depends on the rates. For $L - k \ll L$, a reverse behaviour occurs. If $q < p$, then $z_2 = 1$ and $\langle n_k \rangle$ is flat for $L - k \ll L$. If $q > p$, then $z_2 = q/p$ and $\langle n_k \rangle$ varies with k for $L - k \ll L$. To summarize, one defines two effective roots z_l and z_r for sites near $k = 1$ (the left-hand end) and $k = L$ (the right-hand end), respectively. We then have

$$z_\mathrm{l} = \begin{cases} 1 & q > p \\ q/p & q < p \end{cases} \tag{14}$$

and

$$z_\mathrm{r} = \begin{cases} q/p & q > p \\ 1 & q < p. \end{cases} \tag{15}$$

So there is a phase transition at $p = q = r/2$. This corresponds to $u = v = \bar{s} = \bar{w}$.

If $r = -p - q$, one of the roots of (11) is -1 and the other is $-q/p$. The same behaviour is repeated, that is

$$z_\mathrm{l} = \begin{cases} -1 & -q > -p \\ -q/p & -q < -p \end{cases} \tag{16}$$

and

$$z_\mathrm{r} = \begin{cases} -q/p & -q > -p \\ -1 & -q < -p. \end{cases} \tag{17}$$

Again, there is a phase transition at $p = q = -r/2$. This corresponds to $\bar{u} = \bar{v} = s = w$.

It was seen that on two segments of the boundary of the physical parameter space there exists a static phase transition. These segments ($r = |p + q|$) correspond to cases where the equilibrium state on an infinite lattice without injection and extraction is not unique. On the other segments of the boundary of the physical parameter space ($r = |p - q|$), where the equilibrium state is unique on an infinite lattice without injection and extraction, there is no static phase transition for the lattice with boundaries.

4. The dynamic phase transition of the system

The homogeneous part of (4) can be written as

$$\langle \dot{n}_k \rangle = h_k^l \langle n_l \rangle. \tag{18}$$

The eigenvalues and eigenvectors of the operator h satisfy

$$\begin{aligned} E\ x_k &= -(v+w+u+s)x_k + (v-\bar{v})x_{k+1} + (u-\bar{u})x_{k-1} \qquad k \neq 1, L \\ E\ x_1 &= -(v+w+a+a')x_1 + (v-\bar{v})x_2 \\ E\ x_L &= -(u+s+b+b')x_L + (u-\bar{u})x_{L-1} \end{aligned} \tag{19}$$

where the eigenvalue and the eigenvector have been denoted by E and x, respectively. The solution to these is

$$x_k = \alpha z_1^k + \beta z_2^k \tag{20}$$

where the z_j's satisfy

$$E = -(v+w+u+s) + (v-\bar{v})z + (u-\bar{u})z^{-1} \tag{21}$$

and

$$\begin{aligned} &(v-\bar{v})(\alpha z_1^2 + \beta z_2^2) - (E+a+a'+v+w)(\alpha z_1 + \beta z_2) = 0 \\ &(u-\bar{u})(\alpha z_1^{L-1} + \beta z_2^{L-1}) - (E+b+b'+u+s)(\alpha z_1^L + \beta z_2^L) = 0. \end{aligned} \tag{22}$$

Defining

$$\begin{aligned} \delta a &:= a + a' - (u+s) \\ \delta b &:= b + b' - (v+w) \end{aligned} \tag{23}$$

and using (21) to eliminate E, one arrives at

$$[(u-\bar{u}) + z_1 \delta a][(v-\bar{v})z_2^{L+1} + z_2^L \delta b] - [(u-\bar{u}) + z_2 \delta a][(v-\bar{v})z_1^{L+1} + z_1^L \delta b] = 0. \tag{24}$$

This is the same as equation (15) in [23], with u and v replaced by $u-\bar{u}$ and $v-\bar{v}$, respectively. The qualitative difference between (15) in [23] and (24) is that u and v are non-negative, whereas $u-\bar{u}$ and $v-\bar{v}$ may be negative. Defining

$$\begin{aligned} Z_j &:= z_j \sqrt{\left| \frac{v-\bar{v}}{u-\bar{u}} \right|} \\ A &:= \operatorname{sgn}(u-\bar{u}) \frac{\delta a}{\sqrt{|(v-\bar{v})(u-\bar{u})|}} \\ B &:= \operatorname{sgn}(v-\bar{v}) \frac{\delta b}{\sqrt{|(v-\bar{v})(u-\bar{u})|}} \end{aligned} \tag{25}$$

equation (24) is simplified to

$$Z_2^{L+1}(1 + A\ Z_1)(1 + B/Z_2) - Z_1^{L+1}(1 + A\ Z_2)(1 + B/Z_1) = 0. \tag{26}$$

Using (21), it is seen that

$$z_1 z_2 = \frac{u-\bar{u}}{v-\bar{v}} \tag{27}$$

or

$$Z_1 Z_2 = \operatorname{sgn}[(u-\bar{u})(v-\bar{v})]. \tag{28}$$

The eigenvalue E is also written as

$$\begin{aligned} E &= -(v+w+u+s) + \sqrt{|(u-\bar{u})(v-\bar{v})|}[Z \operatorname{sgn}(v-\bar{v}) + Z^{-1} \operatorname{sgn}(u-\bar{u})] \\ &= -(v+w+u+s) + \operatorname{sgn}(v-\bar{v}) \sqrt{|(u-\bar{u})(v-\bar{v})|}(Z_1 + Z_2) \\ &= -(v+w+u+s) + \operatorname{sgn}(u-\bar{u}) \sqrt{|(u-\bar{u})(v-\bar{v})|}(Z_1^{-1} + Z_2^{-1}). \end{aligned} \tag{29}$$

Let us have a closer look at (26). Using (28), (26) is converted to a polynomial equation for Z_j, having $2L+2$ roots. For $(u-\bar{u})(v-\bar{v}) > 0$, $Z_j = 1$ and $Z_j = -1$ obviously satisfy (26). For $(u-\bar{u})(v-\bar{v}) < 0$, $Z_j = i$ and $Z_j = -i$ are the trivial solutions of (26). However, these solutions lead to

$$x_k = z^k(\alpha + \beta k) \tag{30}$$

not something like (20). And this form for x_k generally does not satisfy the boundary conditions at $k = 1, L$. So the other (nontrivial) $2L$ roots of (26) correspond to the eigenvalues of h.

First consider the case $(u-\bar{u})(v-\bar{v}) > 0$. If all of the roots of Z_j are phases (unimodular), then

$$E \leqslant -(v+w+u+s) + 2\sqrt{(u-\bar{u})(v-\bar{v})}. \tag{31}$$

The equality holds if $Z_j = \mathrm{sgn}(v-\bar{v}) = \mathrm{sgn}(u-\bar{u})$. Normally, this is not a nontrivial root of (26), but in the thermodynamic limit $L \to \infty$ the nontrivial roots of (26) fill the whole unit circle, so the relaxation time for this case is

$$\tau = \left[u+v+w+s-2\sqrt{(u-\bar{u})(v-\bar{v})}\right]^{-1}. \tag{32}$$

It is seen that it does not depend on the injection and extraction rates. If, however, some of the solutions of (26) are not phases, then the situation is different. Let $Z_1 = Z$ be a root of (26) with $|Z| > 1$. In the thermodynamic limit $L \to \infty$, (26) becomes

$$\left(1+\frac{A}{Z}\right)\left(1+\frac{B}{Z}\right) = 0 \tag{33}$$

which has the solutions

$$Z = -A, -B. \tag{34}$$

However, note that we were seeking solutions with moduli greater than one. This shows that there is such a solution provided $|A| > 1$ or $|B| > 1$. If both hold, there exist two solutions with moduli greater than one. Suppose $|A| > 1$. Putting $Z_1 = -A$ in (21), one arrives at

$$E = -(v+w+u+s) - \mathrm{sgn}(u-\bar{u})\sqrt{(u-\bar{u})(v-\bar{v})}(A+A^{-1}). \tag{35}$$

If $\mathrm{sgn}(u-\bar{u})A < 0$, this value of E violates (31), and the relaxation time is no longer obtained from (32). In this case,

$$\tau = \left[v+w+u+s+\mathrm{sgn}(u-\bar{u})\sqrt{(u-\bar{u})(v-\bar{v})}(A+A^{-1})\right]^{-1} \tag{36}$$

which is greater than (32), and does depend on the injection and extraction rates. This is the dynamic phase transition. The point at which this occurs is

$$\delta a = -\sqrt{(u-\bar{u})(v-\bar{v})}. \tag{37}$$

In terms of the injection and extraction rates, the transition point is

$$a + a' = u + s - \sqrt{(u-\bar{u})(v-\bar{v})}. \tag{38}$$

A similar behaviour is seen at the transition point

$$b + b' = v + w - \sqrt{(u-\bar{u})(v-\bar{v})}. \tag{39}$$

If the injection and extraction rates are less than this, then we have

$$\tau = \left[v+w+u+s+\mathrm{sgn}(u-\bar{u})\sqrt{(u-\bar{u})(v-\bar{v})}(B+B^{-1})\right]^{-1}. \tag{40}$$

These sound quite similar to the results of [23], but there is a difference. In the models studied in [23], either A could be less than -1 or B, and it was impossible that both could

be less than one. The reason is that there $s = w = \bar{u} = \bar{v} = 0$, and this means that in the physical region (where all of the rates are non-negative), either the left-hand side of (38) is always greater than the right-hand side of (38), or the left-hand side of (39) is always greater than the right-hand side of (39), since one of the right-hand sides is nonpositive. However, this is not the case in the present model. Defining

$$\begin{aligned} \mathcal{A}_1 &:= u + s - \sqrt{(u-\bar{u})(v-\bar{v})} = \bar{u} + \bar{s} - \sqrt{(\bar{u}-u)(\bar{v}-v)} \\ \mathcal{B}_1 &:= v + w - \sqrt{(u-\bar{u})(v-\bar{v})} = \bar{v} + \bar{w} - \sqrt{(\bar{u}-u)(\bar{v}-v)} \end{aligned} \tag{41}$$

it is seen that at least one of $\mathcal{A}_1$ or $\mathcal{B}_1$ are positive (apart from the special case $u = v = \bar{s} = \bar{w}$ and $\bar{u} = \bar{v} = s = w = 0$, or *vice versa*, where both of them are zero), but it is also possible that both of them are positive. In general, there may be three phases:

$$\tau = \begin{cases} [v + w + a + a' + (u-\bar{u})(v-\bar{v})(a + a' - u - s)^{-1}]^{-1} & \text{region I} \\ [u + s + b + b' + (u-\bar{u})(v-\bar{v})(b + b' - v - w)^{-1}]^{-1} & \text{region II} \\ \left[v + w + u + s - 2\sqrt{(u-\bar{u})(v-\bar{v})}\right]^{-1} & \text{otherwise.} \end{cases} \tag{42}$$

Regions I and II are defined as

$$a + a' < \mathcal{A}_1 \qquad a + a' - b - b' < \mathcal{A}_1 - \mathcal{B}_1 \qquad \text{for region I} \tag{43}$$

$$b + b' < \mathcal{B}_1 \qquad a + a' - b - b' > \mathcal{A}_1 - \mathcal{B}_1 \qquad \text{for region II.} \tag{44}$$

So the system may have two phases or three phases, depending on whether only one of $\mathcal{A}_1$ and $\mathcal{B}_1$ are positive or both of them are positive. In the special case mentioned above, the system has only one phase. This is the same Glauber model at zero temperature with diffusion as studied in [23].

Next consider the case $(u - \bar{u})(v - \bar{v}) < 0$. If all of the solutions to (26) are phases, then (29) shows that

$$\Re(E) = -(v + w + u + s) \tag{45}$$

and from that,

$$\tau = (v + w + u + s)^{-1}. \tag{46}$$

So in this case the relaxation time does not depend on the injection and extraction rates. Moreover, the eigenvalues of h are complex, not real. This means that the relaxation of the system toward its stationary state is oscillatory.

Now suppose that there exist solutions for (26) that are not phases. Let $|Z_1| > 1 > |Z_2|$. At the thermodynamic limit, and using $Z_2 = -Z_1^{-1}$, (26) becomes

$$\left(1 - \frac{A}{Z_1}\right)\left(1 + \frac{B}{Z_1}\right) = 0. \tag{47}$$

The solution to this is

$$Z_1 = A, -B. \tag{48}$$

It is obvious that to have non-phase roots, either $|A|$ or $|B|$ should be greater than unity. Suppose $|A| > 1$. Corresponding to $Z_1 = A$, one obtains

$$E = -(v + w + u + s) - \frac{1}{\delta a}[(\delta a)^2 - |(u-\bar{u})(v-\bar{v})|]. \tag{49}$$

As $|A| > 1$, the expression in the bracket is positive. If $\delta a < 0$, then this value of E is greater than the right-hand side of (45). So this value of E determines the relaxation time. That is,

$$\begin{aligned} \tau &= \{v + w + u + s + (\delta a)^{-1}[(\delta a)^2 - |(u-\bar{u})(v-\bar{v})|]\}^{-1} \\ &= [v + w + a + a' - |(u-\bar{u})(v-\bar{v})|(a + a' - u - s)^{-1}]^{-1}. \end{aligned} \tag{50}$$

A similar argument shows that for $\delta b < -\sqrt{|(u-\bar{u})(v-\bar{v})|}$ the relaxation time is

$$\tau = [u + s + b + b' - |(u-\bar{u})(v-\bar{v})|(b + b' - w - v)^{-1}]^{-1}. \tag{51}$$

Finally, if both $|A|$ and $|B|$ are greater than unity, then the larger of (50) and (51) is the relaxation time. Defining $\mathcal{A}_2$ and $\mathcal{B}_2$ similarly to (41),

$$\begin{aligned} \mathcal{A}_2 &:= u + s - \sqrt{(u-\bar{u})(\bar{v}-v)} = \bar{u} + \bar{s} - \sqrt{(\bar{u}-u)(v-\bar{v})} \\ \mathcal{B}_2 &:= v + w - \sqrt{(\bar{u}-u)(v-\bar{v})} = \bar{v} + \bar{w} - \sqrt{(u-\bar{u})(\bar{v}-v)} \end{aligned} \tag{52}$$

one arrives at

$$\tau = \begin{cases} [v + w + a + a' + (u-\bar{u})(v-\bar{v})(a + a' - u - s)^{-1}]^{-1} & \text{region I} \\ [u + s + b + b' + (u-\bar{u})(v-\bar{v})(b + b' - v - w)^{-1}]^{-1} & \text{region II} \\ (v + w + u + s)^{-1} & \text{otherwise} \end{cases} \tag{53}$$

where the definitions of the regions are the same as (43) and (44), with $\mathcal{A}_1$ and $\mathcal{B}_1$ replaced by $\mathcal{A}_2$ and $\mathcal{B}_2$, respectively. Note that at least one of $\mathcal{A}_2$ and $\mathcal{B}_2$ is positive (apart from the special case $\bar{u} = v = s = \bar{w}$ and $u = \bar{v} = \bar{s} = w = 0$, or *vice versa*, where both of them are zero), but it may be that both are positive. If only one of them is positive, the system has two phases. If both are positive, it has three phases. In the special case mentioned above, the system has only one phase.

One can combine (42) and (53) in a single relation. First, note that (41) and (52) can be combined as

$$\begin{aligned} \mathcal{A} &:= u + s - \sqrt{|(u-\bar{u})(v-\bar{v})|} = \bar{u} + \bar{s} - \sqrt{|(u-\bar{u})(v-\bar{v})|} \\ \mathcal{B} &:= v + w - \sqrt{|(u-\bar{u})(v-\bar{v})|} = \bar{v} + \bar{w} - \sqrt{|(u-\bar{u})(v-\bar{v})|}. \end{aligned} \tag{54}$$

Then we can write

$$\tau = \begin{cases} [v + w + a + a' + (u-\bar{u})(v-\bar{v})(a + a' - u - s)^{-1}]^{-1} & \text{region I} \\ [u + s + b + b' + (u-\bar{u})(v-\bar{v})(b + b' - v - w)^{-1}]^{-1} & \text{region II} \\ \left\{v + w + u + s - 2\Re\left[\sqrt{(u-\bar{u})(v-\bar{v})}\right]\right\}^{-1} & \text{otherwise} \end{cases} \tag{55}$$

where the definitions of the regions are the same as (43) and (44), with $\mathcal{A}_1$ and $\mathcal{B}_2$ replaced with $\mathcal{A}$ and $\mathcal{B}$, respectively.

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