ELSEVIER

Physica A 277 (2000) 455–468

PHYSICA A

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Information potential and transition to criticality for certain two-species chemical systems

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Received 29 January 1999; received in revised form 19 June 1999

Abstract

Using the general results of the stochastic theory of chemical systems, we consider a certain model of chemical reactions with two species, for which it is possible to calculate the first passage time explicitly and study the transition to criticality. Our method uses a non-standard Hamilton Jacobi theory for the master equation, introduced initially by Kubo et al. [J. Stat. Phys. 9 (1973) 51], which leads to solvable Hamiltonian systems. © 2000 Elsevier Science B.V. All rights reserved.

1. Introduction

The stationary state of a general non-equilibrium reaction diffusion system can be analysed in the large volume limit using the information potential defined as $\Phi(x) \sim -(1/V)\log P(x)$ where $P(x)$ is the stationary probability distribution, V is the volume of the system and Φ is what can be called the information potential [1–6]. It is well known [4–6] that Φ satisfies a Hamilton–Jacobi equation, although a non-standard one. In Refs. [5,6], we proved that this large volume approximation of the stationary distribution is better than the more traditional one, given by the usual Fokker–Planck equation (see Refs. [7–9]). This information potential Φ is a non equilibrium state function, whose general properties are studied in Ref. [3]. It would be a free energy (up to temperature) if the stationary state were an equilibrium state. This function is also the relative entropy of a Dirac distribution located at state x with respect to the probability distribution P (see Refs. [10–13]). Moreover in Ref. [3], we study its relation with the

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PII: S0378-4371(99)00429-X

first exit time out of a basin of attraction of a stable state, and so, with chemical rate constants (see also Refs. [14,15] for the case of Fokker–Planck equations). It turns out that the Hamilton–Jacobi equation satisfied by the information potential is not only more appropriate to the analysis of Master equation, but also mathematically simpler than the Hamilton–Jacobi equation derived from the Fokker–Planck equation. In particular, this leads to a general category of chemical models with several degrees of freedom, that can be explicitly solved, whereas, generally, multidimensional chemical systems cannot be solved analytically in the Fokker–Planck approximation.

The model considered in this paper is a modification of a model introduced as an example of a self-organized critical model in Refs. [16–18]. Because this example is explicitly solvable, it is possible to follow the transition to criticality when a certain parameter tends to its critical value, namely, in general, the rate constant is exponentially small of the type $\exp(-VS)$ (V is the volume and S is the regular solution of the Hamilton–Jacobi equation), but when the parameter tends to its critical value, S tends to 0 in the way calculated below.

This article is organized as follows: Section 2 describes the model and its deterministic behavior, Section 3 describes the Master equation, the Hamilton Jacobi equation and the first exit time in terms of the information potential. In Section 4, we solve explicitly the related Hamiltonian equations and in Section 5 we calculate the minimal action. The details of the calculations are given in two appendices. Although we have tried to make this article self-contained, our result is an explicit example of the formalism developed in Ref. [3], to which we refer for general motivation and justification.

2. Deterministic behavior of the model

The model is a variation of the self-organized critical model of Ref. [18]. We consider three species S, R, I, which evolve according to the following reactions:

$$\begin{aligned} &\mathrm{S} \xrightarrow{1} \mathrm{R}\,, \\ &\mathrm{R}+\mathrm{S} \xrightarrow{\alpha} 2\mathrm{S}\,, \\ &2\mathrm{S} \underset{\bar\beta}{\overset{\beta}{\rightleftarrows}} \mathrm{S}+\mathrm{I}. \end{aligned} \tag{2.1}$$

In the metaphor of disease propagation of Ref. [18], S is the sick species, R the normal (or recovering) species and I the immune species. In Ref. [18], we considered only the case $\bar\beta = 0$ and proved that the evolution exhibits a self-organized critical behavior, at least at the deterministic level. This behavior was destroyed in the stochastic approach as was proved in Ref. [18]. The introduction of the inverse reaction with rate $\bar\beta$, allows us to follow the limit when $\bar\beta$ tends to zero. The reactions (Eq. (2.1)) preserve the number S+R+I and if we denote s, r, i the concentration of S, R and I, then the deterministic equations are

$$\frac{ds}{dt} = s(-1 + \alpha r - \beta s + \bar{\beta}(1 - r - s)),$$
$$\frac{dr}{dt} = s(1 - \alpha r) \tag{2.2}$$

with the normalization $s + r + i = 1$.

Assuming that $\alpha > 1$, the stationary points are

(i) all points with $s = 0$,

(ii) the point

$$(r^*, s^*) = \left(\frac{1}{\alpha}, \frac{\bar{\beta}(1 - 1/\alpha)}{\beta + \bar{\beta}}\right). \tag{2.3}$$

We denote

$$a = \frac{\bar{\beta}(1 - 1/\alpha)}{\beta + \bar{\beta}}. \tag{2.4}$$

The stationary point given by Eq. (2.3) lies in the physical region $r + s \leqslant 1$.

An elementary stability analysis of Eqs. (2.2) shows that

(i) the stationary point $(1/\alpha, a)$ is stable

(ii) the points $(r_0, 0)$ are repulsive for

$$r_0 > \bar{r}_0 \equiv \frac{1 - \bar{\beta}}{\alpha - \bar{\beta}} \tag{2.5}$$

and attractive for

$$r_0 < \bar{r}_0.$$

When $\bar{\beta}$ tends to zero, the attractive point $(1/\alpha, a)$ and the separating point $(\bar{r}_0, 0)$ tend together towards the same point $(1/\alpha, 0)$ producing the self-organized criticality. Note also that $\bar{r}_0 < 1/\alpha$. The phase portriat of Eqs. (2.2) is drawn in Fig. 1 and explained in Appendix A. We shall assume henceforth

$$\alpha > \beta + \bar{\beta}. \tag{2.6}$$

3. Master equation and rate constant

The master equation [1–6] describes the evolution of the distribution probability densities $P(r, s, t)$ to find concentrations (r, s) at time t. It has the form

$$\frac{\partial P(r,s,t)}{\partial t} = (\mathrm{LP})(r,s,t),$$

where

$$(\mathrm{LP})\quad (r,s) = \sum_{n,m} \left[w_{nm}\left(r - \frac{n}{N}, s - \frac{m}{N}\right) P\left(r - \frac{n}{N}, s - \frac{n}{N}\right) - w_{n,m}(r,s)P(r,s)\right]$$

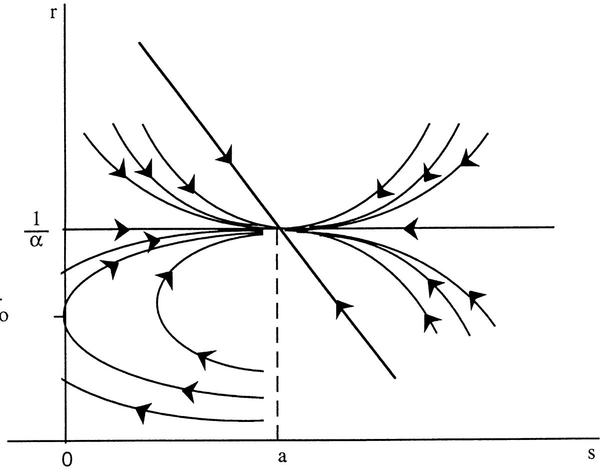

Fig. 1. Phase portrait of the trajecotries of Eqs. (2.2).

and $w_{nm}(r,s)$ is the rate of the transition

$$(r,s) \to \left(r + \frac{n}{N},\ s + \frac{m}{N}\right)$$

corresponding to the reactions which "produce" n particles R and m particles S, where n, m are given positive or negative integers and N is the total number of particles (or the volume of the system).

It is convenient to use the variable (u, v) defined in Eq. (A.1), namely

$$u = -r, \quad v = r + s \tag{3.1}$$

and to write the master equation in terms of these variables. The possible rates in the variables (u, v) are

$$\begin{aligned} &w_{-1,0} = u + v, \quad w_{+1,0} = -\alpha u(u + v)\,, \\ &w_{0,-1} = \beta(u + v)^2, \quad w_{0,1} = \bar{\beta}(1 - v)(u + v)\,. \end{aligned} \tag{3.2}$$

Using the Hamilton–Jacobi method, introduced by Kubo et al. [2], also developed in Ref. [4], we write the stationary solution $P(u, v)$ as

$$P(u, v) \sim U_0 \exp(-NS(u, v))\,, \tag{3.3}$$

where S satisfies the Hamilton–Jacobi equation

$$H\left(u, v, \frac{\partial S}{\partial u}, \frac{\partial S}{\partial v}\right) = 0 \tag{3.4}$$

with

$$H(u, v, p_u, p_v) = \sum_{n,m} w_{n,m}(u, v)[\exp(n p_u + m p_v) - 1] \tag{3.5}$$

and p_u, p_v denote the conjugate momenta of u, v. S can be called the information or stochastic potential. It would be a free energy for an equilibrium system. We study this function in detail in all generality in a further publication [3]. In particular, we show in Ref. [3], that Eq. (3.4) has at most a unique smooth solution up to an additive constant, when the deterministic vector field (i.e., Eqs. (2.2)) has an isolated zero. Moreover, in our case the isolated zero is an attracting point, and by the results of Ref. [3], the smooth solution should have a minimum at that point.

Finally, in Ref. [3], we show that the average of the first passage time of the stochastic process across the line $s = 0$ can be evaluated as

$$T \sim \exp(N \min S(r, 0)) , \tag{3.6}$$

up to a prefactor, the minimum being taken on all possible values of r (or of u) and S is the regular solution of Eq. (3.4) normalized to be zero at the stationary point given by Eq. (2.3). This passage time is also

$$T \sim \lambda_1^{-1} , \tag{3.7}$$

where λ_1 is the first eigenvalue of the Master equation with absorbing boundary condition on the line $s = 0$.

4. Smooth solution of the Hamilton–Jacobi equation

4.1. Equations and solution

The various coefficients of H are given by Eqs. (3.2) and contain $u + v$ in factor. After division by this overall factor the Hamiltonian becomes

$$\begin{aligned}\tilde{H}(u, v, p_u, p_v) = {} & (\exp(-p_u) - 1) - \alpha u(\exp(p_u) - 1) \\ & + \bar{\beta}(1 - v)(\exp(p_v) - 1) + \beta(u + v)(\exp(-p_v) - 1)\end{aligned} \tag{4.1}$$

and we must find a smooth solution of

$$\tilde{H}\left(u, v, \frac{\partial S}{\partial u}, \frac{\partial S}{\partial v}\right) = 0 . \tag{4.2}$$

To find the smooth solution of Eq. (4.2), we take a point (u_0, v_0) close to the stationary point, compute the Hamiltonian trajectory starting from (u_0, v_0) at time 0 and reach (u, v) at a certain time t which has to be calculated, with energy 0. Then we compute the Lagrangian action along this trajectory and in the process, take the limit when (u_0, v_0) tends to the stationary point (see Ref. [2]).

The Hamiltonian system associated to the Hamiltonian $\tilde{H}$ in Eq. (4.1) is

$$\frac{du}{ds} = \tilde{H}_{p_u} = -e^{-p_u} - \alpha u e^{p_u} , \tag{4.3}$$

$$\frac{dv}{ds} = \tilde{H}_{p_v} = -\beta(u + v)e^{-p_v} + \bar{\beta}(1 - v)e^{p_v} , \tag{4.4}$$

$$\frac{dp_u}{ds} = -\tilde{H}_u = \alpha(e^{p_u} - 1) - \beta(e^{-p_v} - 1) , \tag{4.5}$$

$$\frac{\mathrm{d}p_v}{\mathrm{d}s} = -\tilde{H}_v = -\beta(e^{-p_v} - 1) + \bar{\beta}(^{p_v} - 1) . \tag{4.6}$$

This system, Eqs. (4.3)–(4.6), can be solved by quadratures in an explicit manner. We define

$$\psi = \mathrm{e}^{-p_v} - 1, \quad \varphi = \mathrm{e}^{-p_u} - 1 . \tag{4.7}$$

(i) Multiplying Eq. (4.6) by e^{-p_v} we obtain a close equation for ψ:

$$\frac{\mathrm{d}\psi}{\mathrm{d}s} = \beta\psi^2 + (\beta + \bar{\beta})\psi \tag{4.8}$$

which has a general solution depending on a constant C:

$$\frac{1}{\psi(s)} = -\frac{\beta}{\beta + \bar{\beta}} + C\exp(-(\beta + \bar{\beta})s) . \tag{4.9}$$

(ii) Multiplying Eq. (4.5) by e^{-p_u}, we obtain

$$\frac{\mathrm{d}\varphi}{\mathrm{d}s} = \alpha\varphi + \beta\psi(\varphi + 1) . \tag{4.10}$$

We define a function $Z(z)$ by

$$\varphi = Z\psi \tag{4.11}$$

and, using Eq. (4.8), we obtain for Z the linear equation

$$\frac{\mathrm{d}Z}{\mathrm{d}s} + Z(\beta + \bar{\beta} - \alpha) - \beta = 0 \tag{4.12}$$

which has the general solution depending on an arbitrary constant D

$$Z(s) = \frac{\beta}{\beta + \bar{\beta} - \alpha} + D\exp(\alpha - (\beta - \bar{\beta}))s . \tag{4.13}$$

(iii) Finally, Eq. (4.3) for u can be solved explicitly:

$$u(s) = \exp\left(-\alpha\int_0^s \mathrm{e}^{p_u(s')}\,\mathrm{d}s'\right)\left[u(0) - \int_0^s \mathrm{e}^{-p_u(s)'}\exp\left(\alpha\int_0^{s'} \mathrm{e}^{p_u(s'')}\,\mathrm{d}s''\right)\mathrm{d}s'\right] . \tag{4.14}$$

It is not necessary to calculate v, because we need only the trajectory of energy $\tilde{H} = 0$, so that v can be deduced algebraically from this equation.

4.2. Action

The action along a Hamiltonian trajectory with energy $\tilde{H} = 0$ is given by

$$S = \int_0^s (p_u\,\mathrm{d}u + p_v\,\mathrm{d}v) . \tag{4.15}$$

Using the previous results, it is proved in Appendix B that for a trajectory of energy 0

$$p_u\frac{\mathrm{d}u}{\mathrm{d}s} + p_v\frac{\mathrm{d}v}{\mathrm{d}s} = \frac{\mathrm{d}}{\mathrm{d}s}(up_u + vp_v - p_v) - \psi(Z + \beta) . \tag{4.16}$$

Finally the equation $\tilde{H}=0$, permitting to obtain v is equivalent to

$$Z\left(1+\frac{\alpha u}{1+Z\psi}\right)+\beta(u+v)-\bar{\beta}\frac{(1-v)}{1+\psi}=0\,. \tag{4.17}$$

From Eqs. (4.15) and (4.16), we deduce

$$S=(u(s)p_u(s)+v(s)p_v(s)-p_v(s))-(u(0)p_u(0)+p_v(0)-p_v(0)) \\ -\int_0^s \psi(Z+\beta)\,\mathrm{d}s \tag{4.18}$$

which determines S completely, although not in an explicit form. Nevertheless, we shall see below that this expression is sufficient to deduce the first passage time using Eq. (3.6).

5. Calculation of the minimal action on $s = 0$

5.1. Conditions on the trajectory

We consider the action $S(u,v\,|\,u_0,v_0)$ for an Hamiltonian trajectory joining (u_0,v_0) at $t=0$ to (u,v) at $t=t_{\mathrm{f}}$ at energy 0. The unknown are $p_u(0),p_v(0)$ and t_{f}. We are interested, only in $\mathrm{Min}\,S(u,v\,|\,u_0,v_0)$ on $u+v=0$ (which is the line $s=0$), so that $\partial S/\partial u=\partial S/\partial V$ or $p_u(t_{\mathrm{f}})=p_v(t_{\mathrm{f}})$.

The unknown are still the initial momenta and the final time t_{f}, subject to the facts that

$$\tilde{H}=0\,, \tag{5.1}$$

$$u(t_{\mathrm{f}})+v(t_{\mathrm{f}})=0\,, \tag{5.2}$$

$$p_u(t_{\mathrm{f}})=p_v(t_{\mathrm{f}})\,. \tag{5.3}$$

We choose an initial point (u_0,v_0) close to the stationary point, more precisely

$$u_0=-\frac{1}{\alpha}+\varepsilon,\quad v_0=\frac{\bar{\beta}+\beta/\alpha}{\beta+\bar{\beta}}+\xi\,, \tag{5.4}$$

where ε,ξ are small (and will ultimately tend to zero).

For any dynamical quantity X, we abbreviate X_0 (resp. X_f) the value of X at time 0 (resp. time t_f).

5.2. Asymptotics when ε,ξ tend to 0

We consider now a trajectory $(u(t),v(t))$ starting from (u_0,v_0) given by Eqs. (5.4), at energy 0 and sastisfying conditions (5.1)–(5.3), and we study the aymptotic behavior of this trajectory when ε,ξ tend to 0. In Appendix C, we prove that

(i) $t_f\to\infty$,

(ii) $p_u(t),p_v(t)\to 0$ for finite t, uniformly on any finite time interval,

(iii) the quantity $\bar{\psi}_f \equiv e^{-p_{v,f}} - 1$ is 0 if and only if $\bar{\beta} = 0$,

(iv) $u_f = \frac{1-\bar{\beta}+\bar{\psi}_f}{\bar{\beta}-\alpha}$, (Eq. (C.2)).

5.3. The action when ε, ξ tend to 0

We now remark that $u_f p_{u,f} + v_f p_{v,f} = 0$ because $u_f + v_f = 0$, $p_{u,f} = p_{v,f}$, so that the limiting value of the action given by Eq. (4.18) when ε and ξ tend to zero, is

$$S_f = -p_{v,f} - \int_0^\infty \lim(\psi(s)(Z(s) + \beta))\,ds\,. \tag{5.5}$$

It results from Appendix C (Eqs. (C.19) and (C.20)) that

$$S_f = \log(1 + \bar{\psi}_f) - \frac{1}{v}\frac{(1 - \bar{\beta} + \bar{\psi}_f)\,\bar{\psi}_f}{1 + \bar{\psi}_f} + \frac{1 - v}{v}\log(1 + \gamma\bar{\psi}_f)\,, \tag{5.6}$$

where $v = \alpha - (\beta + \bar{\beta})$, $\gamma = \beta/(\beta + \bar{\beta})$.

From Eq. (3.6), we see that the first passage time across the line $s = 0$ is

$$T \sim \exp(NS_f) \quad \text{(up to prefactor)}. \tag{5.7}$$

If $\bar{\beta} = 0$, then $\bar{\psi}_f = 0$ and $S_f = 0$, so that the estimation of Eq. (5.7) breaks down. It will be shown in another article that S_f vanishes as $\bar{\beta}^2$ if $\bar{\beta}$ tends to zero.

5.4. The most probable exit point

The most probable exit point on the line $s = 0$ (or $u + v = 0$) is computed in Appendix C. It is given by

$$r_f = -u_f = \frac{1 - \bar{\psi}_f - \bar{\beta}}{\alpha - \bar{\beta}}\,. \tag{5.8}$$

This is the point of exit of the Hamiltonian trajectory of least action. Note that this is not the point of separation between attracting and repulsive points on the line $s = 0$, which is $(1 - \bar{\beta})/(\alpha - \bar{\beta})$ (Eq. (2.5)).

In the critical limit ($\bar{\beta} \to 0$), this point tends to $1/\alpha$ (in fact, all remarkable points tend to $1/\alpha$) which also becomes the seperation point. This is precisely the situation of self-organized criticality. Furthermore, the exponential behaviour of the exit time T, as given by (3.6), is no more valid, because the minimal action S_f vanishes, so that the undetermined prefactor takes over. This point is examined in Ref. [18], for a similar example, but using a method adapted to that example. The behavior of the prefactor remains to be investigated.

6. Conclusion

Using modification of a model introduced in Ref. [18], we have examined in detail the transition to a critical behavior when a certain parameter (here $\bar{\beta}$) tends to its critical value. The effect which was studied in this work, is the first exit time of a basin of attraction when $\bar{\beta} > 0$. This relaxation time has been calculated as $\exp(VS)$ where V is the volume of the system and S is a minimal action for a non-standard Hamilton–Jacobi theory associated to the large volume limit of the Master equation. In the present case, it turns out that this method not only gives more precise results than the Fokker–Planck equation, but is also mathematically more tractable (the analogue theory for the Fokker–Planck equation would lead to a non-integrable Hamiltonian system). At the critical value of the parameter, this method shows that the action S vanishes, signaling that the relaxation time is not exponentially large, as one expects in a critical situation. This is also a sign that self-organized criticality might occur in these conditions (see Ref. [18]) although a general characterization of self-organized criticality is still missing, from a stochastic point of view. A precise evaluation of the time exactly at criticality as was done for the models of Ref. [18], requires, in general, new methods.

Appendix A. Phase portrait of Eqs. (2.2)

It is convenient to define new variables

$$u = -r, \quad v = r + s \tag{A.1}$$

so that Eqs. (2.2) become

$$\frac{\mathrm{d}u}{\mathrm{d}t} = -s(\alpha u + 1),$$
$$\frac{\mathrm{d}v}{\mathrm{d}t} = s(-\beta(u+v) + \bar{\beta}(1-v))$$

and

$$\frac{\mathrm{d}u}{\mathrm{d}v} = \frac{1+\alpha u}{\beta(u+v) - \bar{\beta}(1-v)} . \tag{A.2}$$

The equilibrium $(r,s) = (1/\alpha,\, a)$ becomes $(u,v) = (-1/\alpha, (\bar{\beta} + \beta/\alpha)/(\beta + \bar{\beta}))$ and we center everything at that point, defining

$$U = u + \frac{1}{\alpha}, \quad V = v - \frac{\bar{\beta} + \beta/\alpha}{\beta + \bar{\beta}} , \tag{A.3}$$

to obtain

$$\frac{\mathrm{d}U}{\mathrm{d}V} = \frac{\alpha U}{\beta U + (\beta + \bar{\beta})V} . \tag{A.4}$$

This has solutions

$$U = 0,$$
$$V = C|U|^{(\beta+\bar{\beta})/\alpha} + \frac{\beta}{\alpha - (\beta + \bar{\beta})} U ,$$

where C is any constant, on coming back to (r,s)

$$r = \frac{1}{\alpha}\,, \tag{A.5}$$

$$s = a + C\left|r - \frac{1}{\alpha}\right|^{(\beta+\bar{\beta})/\alpha} - \left(1 + \frac{\beta}{\alpha - (\beta+\bar{\beta})}\right)\left(r - \frac{1}{\alpha}\right)\,. \tag{A.6}$$

Appendix B. Proofs of certain identites

B.1. Proof of identity (4.16)

We write

$$p_u\frac{\mathrm{d}u}{\mathrm{d}s} + p_v\frac{\mathrm{d}v}{\mathrm{d}s} = \frac{\mathrm{d}}{\mathrm{d}s}(u p_u + v p_v) - \left(u\frac{\mathrm{d}p_u}{\mathrm{d}s} + v\frac{\mathrm{d}p_v}{\mathrm{d}s}\right)\,.$$

Then using Hamilton Eqs. (4.5) and (4.6)

$$\begin{aligned} u\frac{\mathrm{d}p_u}{\mathrm{d}s} + v\frac{\mathrm{d}p_v}{\mathrm{d}s} &= \alpha u(\mathrm{e}^{p_u} - 1) - \beta(u+v)(\mathrm{e}^{-p_v} - 1) + \bar{\beta}v(\mathrm{e}^{p_v} - 1) \\ &\equiv -\tilde{H} + (\mathrm{e}^{-p_u} - 1) + \bar{\beta}(\mathrm{e}^{p_v} - 1)\,. \end{aligned}$$

But $\tilde{H} = 0$, and Eq. (4.6) says that

$$-\bar{\beta}(\mathrm{e}^{p_v} - 1) = -\frac{\mathrm{d}p_v}{\mathrm{d}s} - \beta(\mathrm{e}^{-p_v} - 1)\,,$$

so

$$-\left(u\,\frac{\mathrm{d}p_u}{\mathrm{d}s} + v\,\frac{\mathrm{d}p_v}{\mathrm{d}s}\right) = -\frac{\mathrm{d}p_v}{\mathrm{d}s} - \varphi - \beta\psi = -\frac{\mathrm{d}p_v}{\mathrm{d}s} - \psi(Z+\beta)\,.$$

B.2. Proof of identity (4.7)

$\tilde{H}$ is given by Eq. (4.1). We use the identities

$$\mathrm{e}^{p_u} - 1 = -\frac{\varphi}{\varphi+1} = -\frac{Z\psi}{1+Z\psi},$$

$$\mathrm{e}^{p_v} - 1 = -\frac{\psi}{1+\psi}$$

and equation $\tilde{H} = 0$ reduces to Eq. (4.17) after division by ψ.

Appendix C. Asymptotic of dynamical quantities when ϵ, ξ tend to 0

C.1. Calculation of Z_f, u_f

Because $p_{u,f} = p_{v,f}$ and the definitions given in Eqs. (4.7) and (4.11), we deduce

$$Z_f = 1\,. \tag{C.1}$$

We recall that at any time $\tilde{H}=0$, so that from Eq. (4.17) at time t_f, using Eq. (C.1) and $u_f+v_f=0$

$$u_f=\frac{1+\psi_f-\bar{\beta}}{\bar{\beta}-\alpha}\,. \tag{C.2}$$

C.2. Asymptotic of p_u, p_v, t_f

Until the end of Appendix C, we consider the limits of various quantities when ε and ξ tend to zero.

We take Eq. (4.17) ($\tilde{H}=0$) at time 0 using the values (u_0, v_0) given in Eq. (5.4):

$$0=Z_0\left(1+\frac{\alpha(-1/\alpha+\varepsilon)}{1+Z_0\psi_0}\right)+\beta\left(\frac{(1-1/\alpha)\bar{\beta}}{\beta+\bar{\beta}}+\varepsilon+\xi\right)$$
$$-\left(\frac{\beta\bar{\beta}(1-1/\alpha)}{\beta+\bar{\beta}}-\bar{\beta}\xi\right)\frac{1}{1+\psi_0}\,.$$

After rearrangement

$$0=\psi_0\left[\frac{Z_0^2}{1+Z_0\psi_0}+\frac{\beta\bar{\beta}}{\beta+\bar{\beta}}(1-1/\alpha)\frac{1}{1+\psi_0}\right]$$
$$+\varepsilon\left(\frac{\alpha Z_0}{1+Z_0\psi_0}+\beta\right)+\xi\left(\beta+\frac{\bar{\beta}}{1+\psi_0}\right)\,. \tag{C.3}$$

But $1+\psi_0=\exp(-p_v(0))>0$, $1+Z_0\psi_0=\exp(-p_u(0))>0$ so that Eq. (C.3) forces $\psi_0\to 0$. Then, if $Z_0\psi_0$ does not tend to 0, this would mean $Z_0\to\infty$, which would be in contradiction with Eq. (C.3). So both $p_{u,0}$ and $p_{v,0}$ tend to 0, and Z_0 stays finite.

As a consequence, in Eq. (4.9) for $t=0$, $C\to\infty$ and again from Eq. (4.9) for a finite t,

$$C\to\infty,\ p_v(t)\to 0\quad(\text{finite } t)\,. \tag{C.4}$$

From Eqs. (4.11)–(4.13)

$$\varphi(t)=Z(t)\psi(t)\,,$$
$$Z(t)=D\mathrm{e}^{vt}-\delta,\quad \delta=\frac{\beta}{\alpha-(\beta+\bar{\beta})}\,,$$
$$\psi(t)=\frac{1}{C\mathrm{e}^{-(\beta+\bar{\beta})t}-\gamma},\quad \gamma=\frac{\beta}{\beta+\bar{\beta}}\,,$$
$$v=\alpha-(\beta+\bar{\beta})>0\quad(\text{see Eq. (2.6)})\,. \tag{C.5}$$

Now, $Z_f=1$, by Eq. (C.1), so that

$$D=(1+\delta)\mathrm{e}^{-vt_f}\,. \tag{C.6}$$

If t_f stays finite (when $\varepsilon,\xi\to 0$), then φ and ψ would tend uniformly to 0 and the action would tend to 0 (from Eq. (4.18)).

C.3. Discussion of $u(t)$ and equation for ψ_f

From Eq. (4.14), we need to compute the integral of e^{p_u}. From Eq. (4.5) we have

$$\alpha e^{p_u} = \frac{d p_u}{ds} + \alpha + \beta\psi \,. \tag{C.7}$$

From Eq. (4.8)

$$\frac{d\log\psi}{ds} = \beta\psi + \beta + \bar{\beta} \tag{C.8}$$

and eliminating $\beta\psi$ between Eqs. (C.7) and (C.8), we obtain

$$\alpha e^{p_u} = \frac{d}{ds}(p_u + \log\psi) + v \tag{C.9}$$

so

$$\int_0^t \alpha e^{p_u(s)}\, ds = p_u(t) + \log\psi(t) - p_u(0) - \log\psi(0) - vt \,, \tag{C.10}$$

$$u(t) = \exp(-p_u(t))\exp(p_u(0))\frac{\psi(0)}{\psi(t)}\, e^{-vt}K(t) \,, \tag{C.11}$$

where we have defined

$$K(t) \equiv u_0 - \int_0^t e^{-p_u(s)} \exp\left(\alpha \int_0^s e^{p_u(s')}\, ds'\right) ds$$

and using again Eq. (C.10) in the expression of $K(t)$

$$K(t) = u_0 - \int_0^t e^{vs}\frac{\psi(s)}{\psi(0)} e^{-p_u(0)}\, ds \,. \tag{C.12}$$

Now at $t = t_f$, u_f satisfies Eq. (C.2), so that from Eqs. (C.11) and (C.12), we obtain

$$\frac{1-\bar{\beta}+\psi_f}{\bar{\beta}-\alpha} = \frac{e^{-p_{u,f}} e^{-vt_f}}{\psi_f}\left[\left(-\frac{1}{\alpha}+\varepsilon\right) e^{p_{u,0}}\psi_0 - \int_0^{t_f} e^{vs}\psi(s)\, ds\right]. \tag{C.13}$$

We have $e^{-p_{u,f}} = e^{-p_{v,f}} = \psi_f + 1$ (definition (4.7) of ψ). We shall now take the limit when $\varepsilon \to 0$, $p_{u,0} \to 0$, $t_f \to 0$ and denote by $\widetilde{\lim}$ this limit. Under this limit, it is obvious from Eq. (C.13) that if ψ_f tends to non-zero limit $\bar{\psi}_f$, then $\bar{\psi}_f$ satisfies the identity

$$\frac{1-\bar{\beta}+\bar{\psi}_f}{\bar{\beta}-\alpha} = -\frac{(\bar{\psi}_f+1)}{\bar{\psi}_f}\lim \int_0^{t_f} \frac{e^{-v(t_f-t)}}{Ce^{-(\beta+\bar{\beta})s} - \gamma}\, dt \,.$$

On the other hand, by definition of ψ in Eq. (4.9)

$$\bar{\psi}_f^{-1} = \widetilde{\lim}(Ce^{-(\beta+\beta')t_f} - \gamma)$$

so that $\bar{\psi}_f$ satisfies the following equation:

$$\frac{1-\bar{\beta}+\bar{\psi}_f}{\bar{\beta}-\alpha} = -\frac{\bar{\psi}_f+1}{\bar{\psi}_f}\int_0^{\infty} \frac{e^{-vs}}{(1/\bar{\psi}_f+\gamma)\, e^{-(\beta+\bar{\beta})s} - \gamma}\, ds \,. \tag{C.14}$$

We prove now that $\bar{\psi}_f$ is non-zero. If $\bar{\psi}_f$ were equal to 0, taking Eq. (C.13) we would have

$$\frac{1-\bar{\beta}}{\bar{\beta}-\alpha} = -\frac{1}{\alpha}\widetilde{\lim}\left(\frac{\psi_0}{\bar{\psi}_f e^{\nu t_f}}\right) - \widetilde{\lim}\frac{e^{-\nu t_f}}{\bar{\psi}_f}\int_0^{t_f}\frac{e^{\nu s}}{Ce^{-(\beta+\bar{\beta})s}-\gamma}\,ds\,. \tag{C.15}$$

Because $\bar{\psi}_f \to 0$, $Ce^{-(\beta+\bar{\beta})t_f} \to \infty$, the last limit in Eq. (C.15) is

$$\widetilde{\lim}\frac{e^{-\nu t_f}}{\bar{\psi}_f C}\left(\frac{e^{\alpha t_f}-1}{\alpha}\right) \simeq \frac{1}{\alpha}$$

and so Eq. (C.15) reduces to

$$\frac{1-\bar{\beta}}{\bar{\beta}-\alpha} = -\frac{1}{\alpha}\left(1+\lim\frac{\psi_0}{\bar{\psi}_f e^{\nu t_f}}\right). \tag{C.16}$$

In Eq. (C.16), the limit is a fixed number which is non-zero (to satisfy Eq. (C.16)) so that

$$\widetilde{\lim}\frac{\psi_0}{\bar{\psi}_f e^{\nu t_f}} = \widetilde{\lim}\left(\frac{Ce^{-(\beta+\bar{\beta})t_f}-\gamma}{(C-\gamma)e^{\nu t_f}}\right)$$

but this last term is obviously, 0, so that we have a contradiction and $\bar{\psi}_f$ does not tend to zero.

C.4. Unicity of the solution of Eq. (C.14)

We show that Eq. (C.14) has a unique solution which is $\geqslant -1$, and in fact will be positive if $\bar{\beta} > 0$ and 0 for $\bar{\beta} = 0$.

We rewrite Eq. (C.14) as

$$\frac{1-\bar{\beta}+\bar{\psi}_f}{1+\bar{\psi}_f} = (\alpha-\bar{\beta})\int_0^{\infty}\frac{e^{-\nu s}}{(1+\gamma\bar{\psi}_f)e^{(\beta+\bar{\beta})s}-\gamma\bar{\psi}_f}\,ds\,. \tag{C.17}$$

The function of $\bar{\psi}_f$ in the first number is increasing, while the function of $\bar{\psi}_f$ in the second number is decreasing.

For $\bar{\psi}_f = 0$, the first function takes the value $1-\bar{\beta}$, while the second function takes the value $(\alpha-\bar{\beta})/\alpha > 1-\bar{\beta}$ because $\alpha > 1$, so that there is a unique positive root of Eq. (C.17) for $\bar{\beta} > 0$ and for $\bar{\beta} = 0$ this root is $\bar{\psi}_f = 0$.

C.5. Limit of the action

The limit of action given by Eq. (5.5). But we have

$$\bar{\psi}_f^{-1} = \widetilde{\lim}(Ce^{-(\beta+\bar{\beta})t_f}-\gamma)\,,$$

$$D = (1+\delta)e^{-\nu t_f}, \quad (\text{Eq. (C.6)})\,,$$

so that using Eqs. (4.9) and (4.13)

$$\int_0^\infty \widetilde{\lim}(\psi\ (s)(Z(s)+\beta))\,\mathrm{d}s = \int_0^\infty \frac{(1+\delta)\mathrm{e}^{-\nu s}-(\delta-\beta)}{(1/\bar{\psi}_f+\gamma)\mathrm{e}^{-(\beta+\bar{\beta})s}-\gamma}\,\mathrm{d}s\,. \tag{C.18}$$

Now, using Eq. (C.14) which defines $\bar{\psi}_f$, we have

$$\int_0^\infty \frac{\mathrm{e}^{-\nu s}}{(1/\bar{\psi}_f+\gamma)\mathrm{e}^{(\beta+\bar{\beta})s}-\gamma}\,\mathrm{d}s = \left(\frac{1-\bar{\beta}+\bar{\psi}_f}{\alpha-\bar{\beta}}\right)\left(\frac{\bar{\psi}_f}{1+\bar{\psi}_f}\right)$$

while

$$\int_0^\infty \frac{1}{(1/\bar{\psi}_f+(\gamma)\mathrm{e}^{(\beta+\bar{\beta})s}-\gamma}\,\mathrm{d}s = \frac{1}{\gamma(\beta+\bar{\beta})}\int_0^\gamma \frac{\mathrm{d}u}{(1/\bar{\psi}_f+\gamma)-u}$$
$$= \frac{1}{\gamma(\beta+\bar{\beta})}\log(1+\gamma\bar{\psi}_f)\,,$$

so that using the values $\delta=\beta/[\alpha-(\beta+\bar{\beta})]$, $\gamma=\beta/(\beta+\bar{\beta})$

$$\int_0^\infty \widetilde{\lim}(\psi(s)(Z(s)+\beta))\,\mathrm{d}s = \frac{1}{\nu}\frac{(1-\bar{\beta}+\bar{\psi}_f)\bar{\psi}_f}{1+\bar{\psi}_f} - \frac{1-\nu}{\nu}\log(1+\gamma\bar{\psi}_f) \tag{C.19}$$

and by definition of ψ,

$$p_{v,f} = -\log(1+\bar{\psi}_f)\,. \tag{C.20}$$

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