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**LETTER TO THE EDITOR**

# A simple stochastic model for the dynamics of condensation

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**Abstract.** We consider the dynamics of a model introduced recently by Bialas, Burda and Johnston. At equilibrium the model exhibits a transition between a fluid and a condensed phase. For long evolution times the dynamics of condensation possesses a scaling regime that we study by analytical and numerical means. We determine the scaling form of the occupation number probabilities. The behaviour of the two-time correlations of the energy demonstrates that aging takes place in the condensed phase, while it does not in the fluid phase.

## 1. Introduction

Recently a number of studies have been devoted to the dynamics of the backgammon model, a simple stochastic model which exhibits some of the features of glassy systems such as slow dynamics, non-stationary properties of two-time correlations, violation of the fluctuation-dissipation ratio, etc. [1–8]. The model introduced in [9] is a simple generalization of one of the models defined in [3] (model B), itself closely related to the backgammon model. In contrast with the latter—or with model B—it exhibits, at finite temperature, a phase transition between a fluid and a condensed phase. The aim of this paper is to study the dynamics of condensation in this model, hereafter referred to as model B′. This study is motivated by the fact that, while for model B the non-equilibrium properties such as slow dynamics [3] or aging [5] only occur at zero temperature, here they appear in a whole phase, where the system condenses. In this work we focus our interest on the scaling behaviour of the occupation probabilities and just attempt a short description of the two-time correlations. The dynamics of this model may also serve as a source of inspiration for the understanding of the dynamics of Bose–Einstein condensation, for which little is known. Finally the dynamics of the original branched polymer model introduced by the authors of [9] may have an interest in its own.

## 2. Definitions

Consider a system of $N$ particles distributed amongst $M$ boxes. We denote by $N_i$ the number of particles contained in box number $i$ ($i = 1, \ldots, M$), with $\sum_i N_i = N$. The energy of a given configuration $\mathcal{C} = \{N_1, N_2, \ldots, N_M\}$ of the system is defined as the sum of the energies of individual boxes $\mathcal{E}(\mathcal{C}) = \sum_i E(N_i)$. The Boltzmann factor associated to

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$E(k)$ is denoted by $p_k$. The partition function of the system reads†:

$$Z_{M,N} = \sum_{N_1} \dots \sum_{N_M} p_{N_1} \dots p_{N_M} \delta\left(\sum N_i, N\right) = \oint \frac{\mathrm{d}z}{2\pi\, \mathrm{i} z^{N+1}} [P(z)]^M. \qquad (1)$$

The right-hand expression is obtained by using the integral representation

$$\delta(m, n) = \oint \mathrm{d}z\, z^{m-n}/2\pi\, \mathrm{i}z$$

for the constraint. Equation (1) shows that the equilibrium properties of the system depend only on the set $\{p_k\}$, or, equivalently, on its generating function $P(z) = \sum_k p_k z^k$.

In the present work we restrict our study to the class of models for which $E(k)$ behaves logarithmically‡ for large $k$. The function $P(z)$ has, therefore, a finite radius of convergence $z_c = 1$, with a singularity of the form $(z_c - z)^{\beta-1}$. For definiteness we study model B′ defined by taking $E(k) = \ln(1+k)$, hence $p_k = (1+k)^{-\beta}$, leading to a Dirichlet series for $P(z)$ [9]. In parallel we will recall below the properties of model B [3] defined by taking $E(k) = -\delta_{k,0}$, hence $p_k = \mathrm{e}^{\beta\delta_{k,0}}$ and $P(z) = \mathrm{e}^{\beta} + z/(1-z)$.

## 3. Equilibrium properties

The equilibrium properties of the models follow simply from the previous definitions. In the thermodynamic limit $(M, N \to \infty)$, the density $\rho = N/M$ being fixed, the method of steepest descent can be applied to the integral (1). The saddle-point equation reads $\mathrm{d}P(z)/\mathrm{d}z = \rho P(z)/z$. The saddle-point value $z_s$, which is by definition the thermodynamical fugacity of the model, is thus related to temperature and density. The free energy per box reads $-\beta f = \ln P(z_s) - \rho \ln z_s$. When $z_s$ increases from 0 to $z_c$, $\mathrm{d}f(z_s)/\mathrm{d}z_s = -\ln(z_s)$ is positive; hence $f(z_s)$ is monotonous. One also finds that in this range, $\rho$ increases monotonically from 0 to $\rho_c = z_c P'(z_c)/P(z_c)$. While $\rho_c$ is infinite for model B, it is finite in the case of model B′ as long as $\beta > 2$ and reads $\rho_c = \zeta(\beta-1)/\zeta(\beta)-1$ where $\zeta$ is the Riemann function. This fundamental difference between the two models is a consequence of the behaviour of $p_k$ at infinity and is at the origin of the possible existence of condensation in model B′. Indeed when $\rho_c$ is finite, $f(\rho)$ reaches its maximum at $f(\rho_c) = \ln P(z_c)$. Therefore, as long as $\rho < \rho_c$ the system is 'fluid'. When $\rho > \rho_c$ a condensed phase appears [9]. Thus model B has only a fluid phase for $T > 0$.

These two phases are characterized by different forms of the occupation probabilities, defined as follows. The probability that a generic box, say box number 1, contains $k$ particles is defined as $f_k = \mathrm{Prob}\{N_1 = k\}$, i.e. $f_k$ represents the fraction of boxes containing $k$ particles. The same definition holds out of equilibrium. The conservation of the number of boxes and of the number of particles imposes that $\sum_k f_k = 1$ and $\sum_k k f_k = \rho$. From the definition above, one gets

$$f_k = \sum_{N_1} \dots \sum_{N_M} p_{N_1} \dots p_{N_M} \delta(N_1, k) \delta\left(\sum N_i, N\right) = p_k \frac{Z(N-k, M-1)}{Z(N, M)}. \qquad (2)$$

In the thermodynamic limit, using again the steepest descent method, one obtains

$$f_k = p_k \frac{z_s^k}{P(z_s)} \qquad (\rho < \rho_c) \qquad (3)$$

† Note the difference between the statistics used in equation (1) and that used in the definition of the backgammon model [1, 7, 8]. In contrast to the latter, here the particles are not identified by a label. In this sense they are indistinguishable [3].

‡ Adding to $E(k)$ a linear term in $k$ plays no role because of the constraint.

in the fluid phase. In the condensed phase, one has

$$f_k = \frac{p_k}{P(1)} \qquad (\rho > \rho_c) \tag{4}$$

which is the same as equation (3) with $z_s = 1$. The normalization condition $\sum_k f_k$ is fulfilled by both equations. However, the conservation of the number of particles, $\sum_k k f_k = \rho$, holds only in the fluid phase, while it is violated in the condensed phase where this sum is equal to $\rho_c$. The $M(\rho - \rho_c)$ missing particles sit in a single box [9].

An analogous situation occurs for model B at $T = 0$. Equation (3) gives $f_k = \rho e^{\beta\delta_{k,0}}(1 - z_s)^2 z_s^{k-1}$, with $\rho(1 - z_s) = 1 - f_0$. When $T \to 0$, $\rho_c \to 0$, $z_s \to 1$, hence $f_0 \to 1$. Again, in order to restore the conservation of particles, all the particles have to be in a single box.

## 4. Definition of the dynamics

The rules defining the dynamics of the models follow naturally from their static definitions. These rules were given for model B in [3]. In this work we used both the Metropolis rule, more convenient for Monte Carlo simulations and the heat bath rule, leading to simpler dynamical equations. Let us first describe the former one. At every time step $\delta t = 1/M$ two boxes are chosen at random, a departure box $d$, containing $k$ particles, chosen amongst the non-empty boxes, and an arrival box $a$, containing $l$ particles. Note the difference with the backgammon model, where the departure box is defined by choosing a particle at random (see first footnote on page L20). The transfer of one of the particles from box $d$ to box $a$ is accepted with a probability $\min(1, (p_{k-1}/p_k)(p_{l+1}/p_l))$.

In the heat bath case, once a particle is drawn, it is put into one of the boxes with a probability proportional to the equilibrium probability of the resulting configuration. Thus this move is accepted with a probability

$$\frac{p_{l+1}}{p_l}\left(\sum_{l=0}^{\infty} f_l \frac{p_{l+1}}{p_l}\right)^{-1}.$$

The corresponding dynamical equation for the occupation probabilities is the master equation of a random walk for $N_1$, the number of particles in the generic box number 1:

$$\frac{\partial f_k}{\partial t} = \mu_{k+1} f_{k+1} + \lambda_{k-1} f_{k-1}(1 - \delta_{k0}) - \big(\mu_k(1 - \delta_{k0}) + \lambda_k\big) f_k \tag{5}$$

where $\mu_k = 1$, $(k > 1)$ is the hopping rate to the left, corresponding to $N_1 = k \to N_1 = k - 1$, and

$$\lambda_k = \frac{1 - f_0}{\sum_{l=0}^{\infty} f_l (p_{l+1}/p_l)} \frac{p_{k+1}}{p_k} \qquad (k > 0) \tag{6}$$

is the hopping rate to the right corresponding to $N_1 = k \to N_1 = k + 1$. The factor $1 - \delta_{k0}$ accounts for the fact that one cannot select an empty box as a departure box nor can $N_1$ be negative, i.e. $\lambda_{-1} = \mu_0 = 0$. In other terms a partially absorbing barrier is present at site $k = 0$. This random walk is biased, to the right or to the left, according to whether its velocity $\lambda_k - \mu_k$ is positive or negative, respectively. It is easy to check that equation (5) fulfills both conservations of boxes and particles.

In the stationary state ($\dot{f}_k = 0$) one recovers the equilibrium results given above. The detailed balance condition yields $f_{k+1}/f_k = \lambda_k$, the two possible solutions of which are precisely those given in equations (3) and (4) above, from which one gets

$$\frac{1-f_0}{\sum_{l=0}^{\infty} f_l(p_{l+1}/p_l)} = \begin{cases} z_s & \text{if } \rho < \rho_c \\ 1 & \text{if } \rho > \rho_c. \end{cases} \tag{7}$$

Model B yields

$$\lambda_k = \frac{(1-f_0)\,\mathrm{e}^{-\beta\delta_{k0}}}{1-f_0+f_0\,\mathrm{e}^{-\beta}}. \tag{8}$$

Whatever the value of $\beta$ the walk is biased to the left. Therefore, intuitively, no condensation is expected in this model, except at zero temperature. In this case, since $\lambda_k = 1$ if $k > 0$, and $\lambda_0 = 0$, the system performs a symmetric random walk with a totally absorbing barrier at the origin [3]. Hence for $t \to \infty$, $f_0 \to 1$, i.e. all boxes become empty. Nevertheless, in order to fulfill the conservation of particles, one box has to contain all the particles, as already explained above. $T = 0$ appears thus as a critical point. Let us point out that, for model B, the Metropolis algorithm and the heath bath rule lead to the same dynamical equation for $f_k$.

The case of model B′ is richer. A simple analysis, and a numerical check, show that if $\beta$ is large enough, for small $k$ the bias is to the left, while it is to the right for large $k$. Thus one intuitively expects condensation in this model, for a whole range of values of $\beta$.

## 5. Condensation in the scaling regime

A numerical integration of equation (5), and Monte Carlo simulations for $\beta = 4$ and $\rho = 2 > \rho_c(4) = 0.110$, give some insight into the phenomenology of the dynamics in the condensed phase. Three regimes are observed. First a transient one, with a rapid reorganization of the particles in the boxes, leading to a situation with a fluid part for small $k$ and the appearance of a condensate, i.e. a group of boxes containing a large fraction of the total number of particles. This regime is followed by the scaling regime, our main interest in this work, where the evolution in time of the condensate is self-similar. The number of boxes containing the condensate decreases (although it remains large in this regime).

Finally, at very long times, the condensate reduces to a single box according to a non-universal process where finite size effects should now be taken into account. This sequence of three regimes takes place in a similar fashion in the case of model B. It is also reminiscent of the dynamics of coarsening systems [10].

In order to describe the scaling regime for $f_k$ we set

$$f_k = \begin{cases} \dfrac{p_k}{P(1)}(1+\varepsilon v_k+\cdots) & \text{if } k < u_0/\varepsilon \\ \varepsilon^2 g(u)(1+\mathrm{O}(\varepsilon)) & \text{if } k > u_0/\varepsilon \end{cases} \tag{9}$$

where the small scale $\varepsilon(t)$ is to be determined, and $u = \varepsilon k$ is the scaling variable. $u_0$ fixes the separation between condensed and fluid phases, and corresponds intuitively to the position of the 'dip' clearly visible in figure 1.

The normalization conditions $\sum f_k = 1$ and $\sum k f_k = \rho$ lead, respectively, to

$$\sum_0^{u_0/\varepsilon} \frac{p_k}{P(1)} v_k + \int_{u_0}^{\infty} g(u)\,\mathrm{d}u = 0 \tag{10}$$

and

$$\rho - \rho_c = \int_{u_0}^{\infty} u g(u)\,\mathrm{d}u. \tag{11}$$

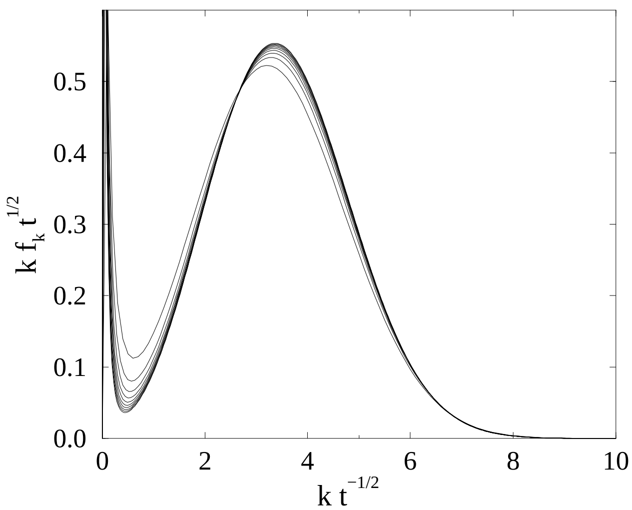


**Figure 1.** Scaling in the dynamics of condensation for model B′. $kf_k\sqrt{t}$, obtained by numerical integration of equation (5), is plotted against $k/\sqrt{t}$ for 10 different times varying from 100 to 1000 ($\rho = 2$, $\beta = 4$).

It is easy to check that, once the limit $t \to \infty$ is taken, with $u_0$ fixed (hence $u_0/\varepsilon \to \infty$), the limit $u_0 \to 0$ can then be taken in (10) and (11).

In order to obtain a continuum description of the master equation we use the expansion, valid when $k$ is large, $p_{k+1}/p_k = 1 - \beta/k + \text{constant}/k^2 + \cdots$. We also set

$$\frac{1 - f_0}{\sum_{m=0}^{\infty} f_m(p_{m+1}/p_m)} = 1 + A\varepsilon + \cdots \tag{12}$$

since this quantity goes to unity for long times. The amplitude $A$ will be determined later.

For small $\varepsilon$ (i.e. large $t$) and fixed $u$ (hence large $k$) one obtains

$$\frac{\dot{\varepsilon}}{\varepsilon^3}(2g + ug') = g'' + \frac{\beta}{u}g' - Ag' - \frac{\beta g}{u^2} + \mathrm{O}(\varepsilon) \tag{13}$$

which is in separable form. The solution for $\varepsilon$ is constant $(t - t_0)^{-1/2}$ or, after a change in the origin of time, $\varepsilon = 1/\sqrt{t}$. In this regime one therefore obtains

$$g'' + \left(\frac{1}{2}u - A + \frac{\beta}{u}\right)g' + \left(1 - \frac{\beta}{u^2}\right)g = 0. \tag{14}$$

This equation is singular at $u = 0$ and $u = \infty$. At $u = 0$ one expects a power singularity for $g$ of the form $u^s$. The Frobenius series $g(u) = \sum_0^{\infty} a_n u^{s+n}$ carried into (14) gives the recursion relation

$$a_{n+2}(s + n + 1)(s + n + \beta + 2) - A(s + n + 1)a_{n+1} + \frac{s + n + 2}{2}a_n = 0 \qquad (n \geqslant -2) \tag{15}$$

with $a_{-1} = a_{-2} = 0$. The radius of convergence of the series thus obtained is infinite. For $n = -2$ one has $(s - 1)(s + \beta) = 0$. Hence, when $u \to 0$, a basis of solutions reads

$$g_1^{(0)}(u) \sim u \qquad g_2^{(0)}(u) \sim u^{-\beta}. \tag{16}$$

Only the first solution may be retained because of the normalization of $g$ (cf equations (10) and (11)). When $u \to \infty$, an asymptotic study of the dominating terms in equation (14)

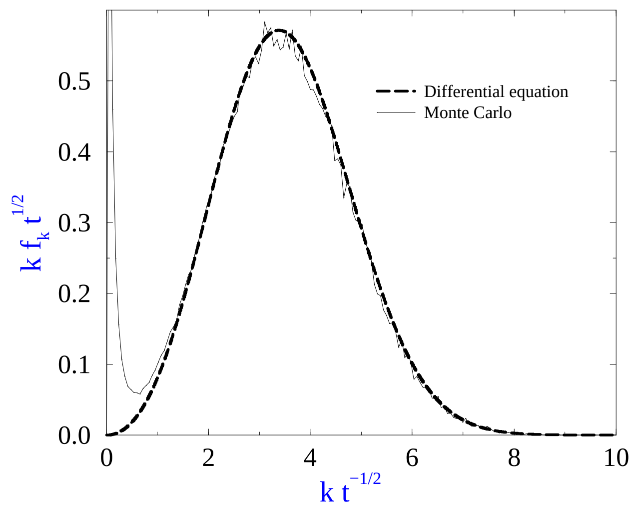


**Figure 2.** Solution of the differential equation (14) with $A = 1.9$, and Monte Carlo simulation ($t = 1000$, $N = 1000$, $M = 500$). ($\rho = 2$, $\beta = 4$.)

leads to another basis of solutions (reminiscent of the particular case $A = \beta = 0$, for which solutions are $u\,e^{-u^2/4}$ and $u\,e^{-u^2/4}\int u^{-2}\,e^{u^2/4}\,du$), namely

$$g_1^{(\infty)}(u) \sim u^{1-\beta}\,e^{-u^2/4+Au} \qquad g_2^{(\infty)}(u) \sim u^{-2}. \tag{17}$$

Again the second behaviour should be excluded, because of the normalization conditions (10) and (11). As the two solutions must be connected,

$$g_1^{(0)}(u) = C_1(A,\beta)g_1^{(\infty)}(u) + C_2(A,\beta)g_2^{(\infty)}(u) \tag{18}$$

and one must impose $C_2(A,\beta) = 0$. This condition determines $A$ as a function of $\beta$. In practice, this may be done numerically either by reconstructing $g$ from its series or directly from a numerical integration of the differential equation (14). The solution of equation (14) may be seen as a continuous deformation of $u\,e^{-u^2/4}$, as $A$ and $\beta$ increase from zero. Note that the solution $g(u) = u\,e^{-u^2/4}$ of the equation $g'' + ug'/2 + g = 0$, corresponding to $A = \beta = 0$, appears also in the scaling regime of model B at $T = 0$, where $f_k = t^{-1}g(kt^{-1/2})$ [3]. Figure 2 displays on the same plot the solution of equation (14) with $A$ determined following this technique, and the Monte Carlo simulation. The agreement between these two curves is excellent. The numerical solution of (5) for large times is hardly distinguishable from the solution of (14).

For theoretical purposes, it may be convenient to cast equation (14) into its Schwarzian form

$$w'' + \frac{1}{2}\left(-\frac{u^2}{8} + \frac{1}{2}Au + \left(\frac{3}{2} - \frac{\beta}{2} - \frac{A^2}{2}\right) + \frac{A\beta}{u} - \frac{\beta(\beta+2)}{2u^2}\right)w = 0 \tag{19}$$

obtained by setting $g = vw$ and choosing $v$ such that no first derivative of $w$ appears in the equation. This leads to

$$g(u) = u^{-\beta/2}\exp\left(-\frac{u^2}{8} + \frac{Au}{2}\right)w(u). \tag{20}$$

Equation (19) may be recognized as a Schrödinger equation with zero energy. Since $w$ is positive, it corresponds to the ground-state solution of the equation. Imposing that the energy of the ground state be zero determines $A$ as a function of $\beta$.

Finally, one may find the explicit form of $f_k$ for small $k$, i.e. in the fluid part of the distribution. Substituting the form (9) for $f_k$ into the master equation (5) leads to

$$\begin{aligned} &v_1 = v_0 + A \\ &p_{k+1}v_{k+1} + p_k v_{k-1} - (p_{k+1} + p_k)v_k = A(p_{k+1} - p_k) \qquad (k > 0) \end{aligned} \tag{21}$$

the solution of which is $v_k = v_0 + kA$. The determination of $v_0$ is made possible by equation (10) which gives

$$v_0 + A\rho_c + \int_0^\infty g(u)\,\mathrm{d}u = 0 \tag{22}$$

where $A$ is already known from above, showing that $v_0$ is negative.

## 6. Two-time correlations of the energy

At $T = 0$, the energy correlation function of model B exhibits aging [5]. It is, therefore, natural to expect the same property for model B′ in the whole low-temperature phase, $\rho$ being fixed. Following the notation of [7], the correlation function of the energy of a generic box, say box number 1, at two times $s$ and $t$ $(s < t)$ reads $c(t, s) = f_0(s)(g_0(t, s) - f_0(t))$, where $g_k(t, s)$ is the probability that box number 1 contains $k$ particles at time $t$, knowing that it was empty at $s$. The evolution in time of this quantity is given by (5), with initial conditions $g_k(s, s) = \delta_{k,0}$. A numerical integration of these equations shows that the normalized correlation function $c(t, s)/c(s, s)$ has the same asymptotic scaling form $\sqrt{s/t}$ as model B [5], for $\beta > \beta_c$, i.e. it exhibits aging in the low-temperature phase. We will come back to the theoretical analysis of this result in a forthcoming publication.

## 7. Discussion

We wish to emphasize the remarkable result obtained in this work, namely that the condensate acquires a universal scaling form directly related to the assumption of a regular power-law behaviour of the $p_k$ at infinity. We checked that the master equation with Metropolis rule led to the same scaling form for $g(u)$. As a consequence of this scaling form, the condensation time behaves as the squared size of the system.

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## References

[1] Ritort F 1995 *Phys. Rev. Lett.* **75** 1190
[2] Franz S and Ritort F 1995 *Europhys. Lett.* **31** 507
[3] Godrèche C, Bouchaud J P and Mézard M 1995 *J. Phys. A: Math. Gen.* **28** L603
[4] Franz S and Ritort F 1996 *J. Stat. Phys.* **85** 131
[5] Godrèche C and Luck J M 1996 *J. Phys. A: Math. Gen.* **29** 1915
[6] Franz S and Ritort F 1997 *J. Phys. A: Math. Gen.* **30** L359
[7] Godrèche C and Luck J M 1997 *J. Phys. A: Math. Gen.* **30** 6245
[8] Kim B J, Jeon G S and Choi M Y 1996 *Phys. Rev. Lett.* **76** 4648
[9] Bialas P, Burda Z and Johnston D 1997 *Nucl. Phys.* B **493** 505
[10] Derrida B, Godrèche C and Yekutieli I 1991 *Phys. Rev.* A **44** 6241