Anomalous coalescence phenomena under stationary regime condition through Thompson’s method

Cláudio Nassif

Departamento de Física, ICEB-UFOP, Morro do Cruzeiro, 35400-000-Ouro Preto-MG, Brazil

Received 15 December 2003; received in revised form 26 January 2004

Abstract

In this work, anomalous coalescence phenomena of type \( A + A \rightarrow A(0) \) are considered in the case of stationary regime, namely the case of an external homogeneous source \( (h) \) of single particles \( A \), in the limit of zero external field rate. The main purpose here is to pick up new critical exponents in the stationary regime for the phenomenon of anomalous coalescence of bubbles found in one-dimension by Josserand and Rica (JR) (Phys. Rev. Lett. 78 (1997) 1215). The critical exponents of statical concentration \( (\delta) \), relaxation time \( (\Delta') \) and the exponent for concentration decay \( (\xi) \) are evaluated in the limit \( h \rightarrow 0 \) (zero field rate). We show that such critical exponents depend on the parameter \( \gamma \) (Physica A 334 (2004) 335), which characterizes the anomalous diffusion condition. In order to explain the anomalous coalescence of JR’s work as already made before by the present author (Physica A 334 (2004) 335), the parameter \( \gamma \) must display an explicit dependence on the dimensionality \( [\gamma = \gamma(d) = 4/d \text{ for } d \leq 2] \). We use such a result \( [\gamma(d)] \) in order to pick up new critical exponents for the special case of anomalous coalescence found by JR (we find \( \delta = 5, \Delta' = \frac{4}{5} \) and \( \xi = \frac{1}{4} \) in 1-d). We also verify that the known scaling relations among such critical indexes (Phys. Rev. A 32(2) (1985) 1129) are obeyed, so that in the special case of \( \gamma = 2 \) (brownian diffusion condition given to mean field regime), we naturally recover those results previously obtained by Rácz (Phys. Rev. A 32(2) (1985) 1129).

We go further to give a better explanation for such new results, taking into account another exponent \( \alpha \) (Physica A 334 (2004) 335) to explain the behavior of diffusion constant, which depends on concentration \( (D = D_0 \langle n \rangle^\alpha) \), that is to say, we obtain analytically new critical indexes which control the diffusion behavior \( (D) \) for long-time regime, in the presence of an external homogeneous source.

© 2004 Elsevier B.V. All rights reserved.

PACS: 64.60; 82.40.—g; 05.10.Cc

Keywords: Anomalous coalescence; Stationary regime; Critical exponents; Thompson’s approach

E-mail address: cnassif@fisica.ufmg.br (C. Nassif).
1. Introduction

Motivated by the possible relevance of understanding the behavior of $A + A \rightarrow A(0)$ brownian diffusion-limited reactions in the stationary regime, Rácz [3] has obtained critical exponents, namely the exponent $\delta$ of statical concentration $n_h$ ($n_h \sim h^{1/\delta}$), the critical dynamical exponent $A'$ for the relaxation time ($\tau \sim h^{-A'}$) and the exponent for the concentration decay $\xi$ ($n \sim \tau^{-\xi}$), being all these quantities evaluated in the limit of zero-field rate ($h \rightarrow 0$), where $h$ represents a non-local homogeneous external source of single particles $A$. Specially for dimension $d = 2$, Rácz [3] found $\delta = 2$, $A' = \frac{1}{2}$ and $\xi = 1$.

On the other hand, motivated by Josserand and Rica’s work (hereafter, JR) [1] and also by a more recent paper [2], where droplet and bubble anomalous coalescence in 1-d was well explained through Thompson’s scaling approach [4], we must be able to pick up anomalous exponents which depend on parameter $\gamma$ for anomalous diffusion condition [5]. We also have to consider $\gamma$ depending on dimensionality ($\gamma(d)$) [2]. So we finally have anomalous critical exponents which could describe the behavior of the stationary regime for the case of anomalous coalescence found by JR.

Thompson [4] proposed a simple heuristic method as a means to study the critical behavior of a system undergoing second-order phase transition. He started from a Landau–Ginsburg–Wilson free energy or hamiltonian, and was able to get an explicit relation for the correlation length critical exponent ($\nu$) as a function of the lattice dimensionality ($d$). If one accepts that this $\Phi^4$-theory is within the same class of universality of the Ising model, Thompson’s work reproduces the exact results for $\nu(d = 2) = 1$ and $\nu(d = 1) \rightarrow \infty$.

Let us enumerate some applications of Thompson’s method. First, we have the evaluation of the correlation length critical exponent of the Random Field Ising Model by Aharony et al. [6] and by Silva [7]. Thompson’s method was also used to evaluate the correlation critical exponent of the $N$-vector model [8]. Yang–Lee edge singularity critical exponents [9] have also been studied by this method. Furthermore, we can mention that such a heuristic approach was recently applied to the critical dynamics of the Ising model [10]. In two recent works [11,12], it was applied to study the special cases of diffusion limited chemical reaction of type $A + B \rightarrow 0$ with equal [11] and different [12] initial concentrations of the two-species. Actually, it is important to mention that there are a great variety of chemical reactions where the diffusion mechanism is responsible for the deviation of mean field-like behavior [13–24].

In a previous work, the renormalization group (RG) method was applied to study brownian diffusion-limited reactions of the type $kA \rightarrow lA$ ($l < k$) by Peliti for the case $k = 2$ [25]. Peliti [25] used a field-theory formulation for this case. He was able to confirm the conjectured decaying exponent, and also demonstrated that the reactions $A + A \rightarrow 0$ and $A + A \rightarrow A$ are within the same universality class with regard to the decaying exponent and the upper critical dimension.

A more recent work by applying RG to these systems of coalescence ($kA \rightarrow lA$) includes that of Ohtsuki [26] and Lee [27]. Lee used the RG calculation for $kA \rightarrow 0$ reaction. He obtained the upper critical dimension $d_c$ of this system, the density decaying at lower dimensions and at $d = d_c$, and also the reaction rate. This formalism
was immediately generalized by Lee [27] to the reaction \( kA \rightarrow lA \) \((l < k)\), so that this model leads to the same density exponent for the case \( kA \rightarrow 0 \), but the amplitude is modified. Here we can also mention the work by Grynberg et al. [28], where multiparticles reactions were studied [28].

Referring to recent work, we can mention Alcaraz et al. [29] who have discussed the interplay among reaction–diffusion processes, critical dynamics and quantum chains. On the other hand, Oliveira [30] has provided a derivation of the exact density profile of a one-dimensional reaction–diffusion process where hard-core particles, subject to diffusion, can be annihilated and created. Another work by Oliveira [31] treated the long-time behavior of an one-species reaction–diffusion process in a hypercubic lattice where a specified number of particles coalesce into a smaller number of them. Following this line of research, we mention again the work of Lee [27], where the brownian diffusion-controlled reaction \( kA \rightarrow 0 \) was treated by applying the RG approach. The RG formalism has been considered a powerful tool to study a large class of reaction–diffusion models [32,33].

Albuquerque and Lyra [34] investigated numerically the kinetics of diffusion-limited annihilation reactions in disordered binary square lattices where the reacting particles are constrained to diffuse on a concentration \( \rho \) of lattice sites. The diffusion-limited annihilation (DLA) models were well explored by many ways. First we can mention the work of Krug [35], where he considered a term of local input rate to be introduced into the diffusion equation, in order to represent DLA phenomena, in the presence of such a local source \((H_0\delta(r))\) [35], being \( H_0 \) a constant. Here we also can mention other kinds of annihilation models, as for instance, the ballistic annihilation. There a great variety of models which are governed by ballistic kinetics [36–41] and also by fractality [42–44]. We could even mention several works by treating coalescence and annihilation processes [45–50], the reactions of type \( nA + mB \rightarrow C \) [51] and others [52–63].

Thompson’s method is a simple alternative way to the RG scheme and has been shown to be a good description for the long-time (long wavelength) regime.

2. The critical exponents in the stationary regime for \( A + A \rightarrow A(0) \) anomalous coalescence

In this section, we study the coalescence reaction model \((A + A \rightarrow A(0))\) with anomalous diffusion condition. This system (lattice) is submitted to an external homogeneous source \((h = \text{constant})\) of particles \( A \). So we suggest that the limit of “zero-field rate” \((h \rightarrow 0)\) may be considered as a critical point [3]. Consequently, near this point \((h \rightarrow 0)\), we are able to extract the following critical exponents: \( \delta(h \rightarrow 0) \), that is a statical critical exponent for the concentration in stationary regime; \( A'(\tau_h \sim h^{-A'}) \), that is a dynamical critical exponent for the relaxation time \( \tau_h \), obtained in the limit of “zero-field rate”; and finally the exponent \( \xi \) [3], which represents the exponent for the concentration decaying.

According to a previous paper [2], an effective action to describe \( A + A \rightarrow A(0) \) coalescence with anomalous diffusion condition was proposed by the present author,
namely
\[ A_\gamma = \int d^d r \left[ \frac{1}{2} D (\nabla^{\gamma/2} n)^2 - H n + \frac{1}{3} K n^3 + \frac{1}{2} \frac{\partial (n^2)}{\partial t} \right], \tag{1} \]

where \( k \) represents the reaction rate; \( D \) represents the diffusion constant; \( \gamma \) is a parameter related to anomalous (enhanced) diffusion [5], and \( H \) is related to a source given by a local distribution function of type \( H = H_0 \delta(r) \), according to Krug’s model [35]. \( H_0 \) is a constant.

In order to understand the meaning of the terms of the action (1), we need to obtain a diffusion differential equation. To do this, we impose the condition \( \delta A_\gamma = 0 \) for constant \( t \) [5], obtaining the following equation of motion:
\[ \frac{\partial n(r,t)}{\partial t} = D \nabla^{\gamma} n + H_0 \delta(r) - K n^2, \tag{2} \]

where \( n \) is the concentration of species \( A \). “\( H_0 \delta(r) \)” stands for a local input rate (a local source) introduced by Krug [35] for the continuous approximation of \( A + A \rightarrow 0 \) reaction (DLA model [35]).

The parameter \( \gamma \) specifies anomalous diffusion behavior. If \( \gamma < 2 \), we have superdiffusion condition. If \( \gamma > 2 \), we have subdiffusion condition. For the special case \( \gamma = 1 \), we get ballistic kinetics [5].

The fractional differential equation above suggests us a non-locality property due to the fractional derivative [64,65] which causes anomaly in diffusion for such cases of coalescence reactions.

In order to treat (1) above, we proceed in an analogous way to Thompson’s reasoning [4], which states the following scaling assumption for each term of the action above. First term:
\[ \left| \int d^d r \left[ \frac{1}{2} D (\nabla^{\gamma/2} n)^2 \right] \right| \sim t^{d-\gamma} \langle n^2 \rangle \sim 1 \tag{3} \]

so that the mean squared value of \( n(\langle n^2 \rangle) \) behaves as
\[ \langle n^2 \rangle \sim t^{\gamma-d}. \tag{4} \]

For the fourth term in (1) we have
\[ \left| \int d^d r \left[ \frac{1}{2} \frac{\partial (n^2)}{\partial t} \right] \right| \sim \langle \Omega \rangle \langle n^2 \rangle t^d \sim 1, \tag{5} \]

where we have considered that
\[ n(t) = n_0 \exp(-\Omega t). \tag{6} \]

By putting (4) into (5), we obtain
\[ \langle \Omega \rangle^{-1} \equiv \tau \sim t^{\gamma}. \tag{7} \]

We observe that (7) points out to the signature of the non-brownian character of these diffusion limited reactions. For \( \gamma = 2 \), we recover the brownian condition.

For the second term in (1) we get the following scaling behavior:
\[ \langle n \rangle \sim t^{-d} \sim \tau^{-d/\gamma}. \tag{8} \]
For the third term in (1), making the plausible hypothesis \( \langle n^3 \rangle \sim \langle n^2 \rangle \langle n \rangle \) [5] (bilinear interaction), and by using (4) and (8) above, we obtain
\[
\langle K \rangle \sim l^{d-\gamma} \sim (l)^{d/\gamma-1} \sim \tau^{d/\gamma-1} \sim \tau^{d/d_e-1},
\]
where
\[ d_e = \gamma. \tag{9} \]

The mean field equation for such reactions is the following:
\[
\frac{\partial n}{\partial t} = -Kn^2
\]
whose solution is \( n \sim t^{-1} = t^{-\xi} \) (\( \xi = 1 \): mean field regime \( d > d_e \)). For \( d < d_e \), the behavior of the density is conjectured on the basis of scaling arguments [66,67] and rigorous bounds [68]. Exact results are given for \( d = 1 \) [69–72].

Now by considering an external homogeneous source \( h \), we write:
\[
\frac{\partial n}{\partial t} = h - Kn^2.
\] \tag{12}

In the mean field regime, we have \( K \sim constant \) [5]. However, let us think in terms of an effective reaction rate \( K_{eff} \), which depends on the dimensionality \( d \) of the lattice, i.e., \( K_{eff} = K(d) \), and thus, let us introduce this information into Eq. (12), obtaining an effective equation which also includes regimes out of mean field behavior, namely
\[
\frac{\partial n}{\partial t} = h - K_{eff}n^2.
\] \tag{13}

In the stationary regime \( \frac{\partial n}{\partial t} = 0 \), we obtain from (13)
\[
h - K_{eff}(\bar{n})^2 = 0. \tag{14}
\]

Now, by considering the scaling result (9) to be the effective reaction rate \( K(d) \), and by introducing (8) \( l \sim n^{-1/d} \) into (9), yields
\[
K_{eff} = \Gamma_0 n^{\gamma/d-1},
\] \tag{15}
where \( \Gamma_0 \) is a proportionality constant.

Finally, by putting (15) into (13), and also by considering the stationary regime condition given in Eq. (14), we obtain
\[
\bar{n} = \left( \frac{h}{\Gamma_0} \right)^{\gamma/d} \sim h^{1/\delta},
\] \tag{16}
where we pick up
\[
\delta = \delta(d, \gamma) = \frac{(d + \gamma)}{d}. \tag{17}
\]

On the other hand, in the case of anomalous diffusion condition, we have obtained the scaling behavior \( \tau \sim l^{\gamma} \sim n^{-\gamma/d} \), being \( l \sim n^{-1/d} \) (from relation (8)). From this scaling result, we can also write
\[
n \sim \tau^{-d/\gamma} = \tau^{-\xi},
\] \tag{18}
where \( \xi = d/\gamma \) means the exponent of concentration decaying.
Now, by introducing (18) above into (15) and into (13), from (14) we finally get
\[
\tau = \tau_h = \left( \frac{h}{T_0} \right)^{-\gamma(d+\gamma)} \sim h^{-\Delta'},
\] (19)
where we obtain
\[
\Delta' = \Delta'(d, \gamma) = \frac{\gamma}{(d + \gamma)}.
\] (20)

It is important to observe that we get \(\xi = 2\), \(\xi' = \frac{1}{2}\) and \(\xi = 1\) when we make \(d = 2\) and \(\gamma = 2\) in (17), (20) and (18), respectively. Indeed we are able to recover Rácz’s exponents [3] as special cases for the stationary regime under brownian diffusion condition.

3. Critical exponents for JR’s anomalous coalescence: scaling relations among such new exponents

In a previous paper [2], we took \(n\) as being the density of particles \(A\) to represent bubbles (or domain) concentration [1], which behaves like \(n \sim t^{-d/\gamma}\), according to (8). \(\gamma\) was considered to be a free parameter. However, it was assumed that \(\gamma\) must be a function of the dimensionality (\(\gamma(d)\)), through the following ansatz [2], namely:

\[
\gamma = \gamma(d) = \begin{cases} 
2, & d \geq 2, \\
\frac{4}{d}, & d \leq 2.
\end{cases}
\] (21)

It must be stressed that the critical exponents \(\delta\), \(\Delta'\) and \(\xi\), which were obtained in the last section (relations (17), (20) and (18)) are functions of the free parameter \(\gamma\). However, now we are interested to pick up such exponents for the special case of the JR’s anomalous result. So in order to do that, we must take into account the ansatz (21). Thus by introducing (21) into (17), (20) and (18) (\(\xi = 1\), for \(d \geq 2\) [2]), we finally obtain the following special exponents:

\[
\delta = \delta(d) = \begin{cases} 
(d + 2), & d \geq 2, \\
\frac{d^2 + 4}{d^2}, & d \leq 2,
\end{cases}
\] (22)

\[
\Delta' = \Delta'(d) = \begin{cases} 
\frac{2}{(d + 2)}, & d \geq 2, \\
\frac{4}{(d^2 + 4)}, & d \leq 2
\end{cases}
\] (23)
and
\[
\xi = \begin{cases} 
1, & d \geq 2, \\
\frac{d^2}{4}, & d \leq 2.
\end{cases}
\] (24)
Here the novelty occurs when we make \( d = 1 \) above. So we get \( \delta = 5, A' = \frac{4}{3} \) and \( \xi = \frac{1}{4} \). Such new results represent the anomalous critical exponents given in stationary regime for JR’s model [1]. Here it is also important to stress that such new exponents [(22)–(24)] even obey the following scaling relations given by Rácz [3], namely: \( A' + 1/\delta = 1 \) and \( \xi A' = 1/\delta \).

4. An interpretation for critical exponents in the case of JR’s coalescence

In a previous work [2], we have considered a diffusion constant \( (D = D_0 \langle n \rangle^x) \) to be put into an effective action \( A_x \) which replaced the description provided by the exponent \( \gamma \). Actually these two descriptions are equivalent [2]. Thus we wrote the following equivalent action, namely:

\[
A_x = \int d^d r \left[ \frac{1}{2} D_0 \langle n \rangle^x (\nabla n)^2 - Hn + \frac{1}{3} Kn^3 + \frac{1}{2} \frac{\partial \langle n^2 \rangle}{\partial t} \right].
\] (25)

\( D_0 \) is a constant. \( \langle n \rangle \) means average concentration on the scale \( l \).

From the first term of (25), by applying the first assumption of Thompson [4], we get the following scaling relation:

\[
\langle n \rangle^x \langle n^2 \rangle^{d-2} \sim 1.
\] (26)

For the fourth term we obtain

\[
\frac{\langle n^2 \rangle^l}{\tau} \sim 1.
\] (27)

From the second term we get

\[
\langle n \rangle^l \sim 1 \Rightarrow l \sim \langle n \rangle^{-1/d}.
\] (28)

We have \( \tau \sim \bar{r} \), and then by comparing (26) with (27), we obtain

\[
\langle n \rangle^x \sim l^{2-\gamma} \Rightarrow l \sim \langle n \rangle^{x/2-\gamma}.
\] (29)

For \( \gamma = 2 \), we have \( x = 0 \) (mean field regime).

By comparing (29) with (28), thus we obtain the following relation by the equality of their exponents, namely

\[
x = \left( \frac{\gamma - 2}{d} \right) \Rightarrow \gamma = xd + 2.
\] (30)

Relation (30) allows us to relate \( \gamma \) to the equivalent exponent \( x \), which defines the diffusion “constant” \( (D = D_0 \langle n \rangle^x) \). Then, starting from the exponent \( x \) instead of \( \gamma \), we are able to give an interpretation to a better understanding the meaning of such critical exponents, in the special case of anomalous coalescence found by JR [1] in 1-d. So in order to do that, firstly we must replace \( \gamma \) in relations (17), (20) and (18), by its equivalent form (30). Therefore we write the following exponents in an equivalent way, namely

\[
\delta = \delta(d, x) = \frac{(d + 2) + xd}{d}.
\] (31)
\[
A' = A'(d, x) = \frac{2 + xd}{(d + 2) + xd}
\] 
(32)

and
\[
\xi = \frac{d}{2 + xd}.
\]
(33)

In the special case \(d = 1\), we say that JR’s anomalous coalescence leads to \(x = 2\) (or \(\gamma = 4\)) \(\Rightarrow \delta = 5, A' = \frac{4}{5}\) and \(\xi = \frac{1}{4}\), according to (31), (32) and (33). Now, finally, we can interpret this fact as follows: In \(d = 1\), for long-time regime, we find lower densities of bubbles, which naturally lead to a weakening of diffusion rate since we have \(D = D_0 \langle n \rangle^2\) [2], where \(\langle n \rangle\) is very low in such a regime. Of course this weakening of diffusion represents a kind of subdiffusion (\(\gamma = 4\)), which leads to a slower decaying of concentration \((n \sim t^{-1/\gamma} = t^{-1/4})\). Consequently, in this anomalous condition, and for stationary regime, where we have the presence of an external source \((h)\) of single species \(A\), the critical limit \(h \to 0\) leads to the following anomalous behavior: \(n_h \sim h^{1/5}\) and \(\tau_h \sim h^{-4/5}\). This means that the statical concentration behavior \(n_h\) has a slower decaying and \(\tau_h\) (relaxation time behavior) has a faster increasing.

5. Conclusions and prospects

In this paper, the diffusion-controlled reactions of type \(A + A \to A(0)\) with anomalous coalescence were considered in the case of a stationary regime, namely the case of an external homogeneous source \((h)\) of single particles \(A\) for long-time regime, in the limit of zero external field rate. Then we were able to pick up new critical exponents in the stationary regime for the phenomenon of anomalous coalescence of bubbles found in one-dimension by Josserand and Rica (JR) [1]. The new critical exponents of statical concentration \((\delta)\), relaxation time \((A')\) and the exponent for concentration decaying \((\xi)\) were evaluated in the limit \(h \to 0\) (zero field rate). We have shown that such critical exponents depend on parameter \((\gamma)\), which characterizes the anomalous diffusion condition. Here, the parameter \(\gamma\) have displayed an explicit dependence on the dimensionality \((\gamma = \gamma(d) = 4/d\) for \(d \leq 2\)) [2]. We have used such a result \((\gamma(d))\) in order to pick up new critical exponents for the special case of the anomalous coalescence found by JR. We also have shown that the known scaling relations among the critical indexes are obeyed, so that, in the special case of brownian condition given in mean field regime, we naturally recover those results previously obtained by Rácz [3]. We also gave an interpretation for such new results, taking into account another exponent \((x)\), which controls the behavior of diffusion “constant” through the concentration \((D = D_0 \langle n \rangle^2)\).

In the future we will use the present method to study field theories described by Grassmann fields. There we aim to work out, for instance, the \(\overline{QED}_4\) running coupling constant dependence on the energy scale. The scalar theories-\(\Phi^n\) were already studied by the present method [73]. We were able to pick up \(\beta\)-functions [73] for such theories, namely the running coupling constant dependence on the energy scale.
Thompson’s approach also seems to be appropriated to study various features of the growth of a polymer chain. As Thompson’s method is essentially a scaling approach, it can be employed in this task as an alternative way to the RG formalism.

References