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Anomalous coalescence from a nonlinear Schroedinger equation with a quintic term: interpretation through Thompson's approach

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Abstract

Inspired by models for $A+A \rightarrow A(0)$ reactions with non-Brownian diffusion, we suggest a possible analytical explanation for the phenomena of anomalous coalescence of bubbles found in one-dimension (1d) by Josserand and Rica through numerical work [Phys. Rev. Letters 78 (1997) 1215]. The explanation firstly requires an exponent γ, which is sometimes used to describe anomalous diffusion. Here it displays an explicit dependence on the dimensionality ($\gamma=\gamma(d)=4/d$ for $d \leqslant 2$). So we have $d_c=2$, coinciding with the upper critical dimension of $A+A \rightarrow A(0)$ reactions (Mod. Phys. Lett. B 13 (1999) 829; Mod. Phys. Lett. B 15(26) (2001) 1205) with Brownian diffusion condition ($\gamma=2$). Thus anomalous coalescence emerges, only below the critical dimension ($d<2$). We show that the typical size of the structures (bubbles) grows as $R(t) \sim t^{1/4}$ in 1d. An alternative explanation could also be thought as a diffusion constant D which depends on the average concentration ($\langle n \rangle$), namely $D=D_0\langle n \rangle^{\alpha}$. It is introduced into an effective action for $A+A \rightarrow A(0)$ reactions. Therefore we are also able to reproduce the anomalous behavior for $n(t)$ and $R(t)$ in 1d, being $\alpha=0$ for $d \geqslant 2$ (mean field behavior) and $\alpha=2(2-d)/d^2$ for $d \leqslant 2$.

Keywords: Thompson's approach; Anomalous coalescence; Nonlinear Schrödinger equation

1. Introduction

Motivated by the possible relevance on understanding superfluid He_4 cavitation, filamentation on nonlinear optics and Bose–Einstein condensation in Li_7, Josserand and

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Rica (JR) [1] have studied the nonlinear Schroedinger equation (NLSE) with the addition of a quintic term. As pointed out by them [1], the physical behavior observed in their numerical investigation is very analogous to the formation of droplets in a "dynamical" first-order phase transition. The starting point of JR [1] is the NLSE

$$i\,\frac{\partial \Psi}{\partial t} = -\frac{1}{2}\,\nabla^2\Psi - 2\rho_c|\Psi|^2\Psi + |\Psi|^4\Psi \,. \tag{1}$$

In (1) $|\Psi|^2$ is the order parameter and ρ_c is related to the critical density for cavitation, that is, when the sound speed vanishes. When $|\Psi|^2 \approx \rho_c$, the presence of the quintic term in (1) is necessary, and when $|\Psi|^2 \ll \rho_c$, it can be neglected.

As noticed by JR, the rich dynamics which emerges from the numerical analysis of (1) develops itself in three stages. In the first one, starting from an initial uniform density ρ_o slightly less than ρ_c, density variations grow exponentially in time, creating a cellular modulation with length scale of the fastest growing mode. As pointed out by JR, this very short scale modulation expels matter from one domain to another, creating regions with more stable densities, and leading to a splitting of space onto well-defined domains with large ($\sim\rho_c$) and small (~ 0) stable densities. The second intermediary stage is short in time: the pressure difference between the low density (gas) and the large density (liquid) phases contracts the liquid phase, until the liquid density reaches $\frac{3}{2}\rho_c$, the point where pressure equilibrium is established. Finally JR observed a third stage, with slow spatiotemporal dynamics, where the stable droplets and bubbles coalesce. Trying to understand this last step, JR wrote a rate equation (mean field-like) to describe the time evolution of the number of bubbles. However the mean field equation has failed in describing the observed behavior. We think that an appropriate rate equation limited by an anomalous diffusion could overcome this difficulty. The present paper will address the understanding of JR's third step, in order to explain droplets and bubbles anomalous coalescence in 1d through Thompson's scaling approach [2].

In 1976, Thompson [2] 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 (ν) as a function of the lattice dimensionality (d). If one accepts that this Φ^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 $\nu(d=1)\to\infty$.

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. [3] and by one of the present authors [4]. Thompson's method was also used to evaluate the correlation critical exponent of the N-vector Model [5]. Yang–Lee edge singularity critical exponents [6] 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 [7]. In a more recent paper [8], it was applied to study the diffusion limited chemical reaction $A+B\to 0$ with different initial concentrations of the two species. Anomalous diffusion conditions are also considered [9,10] by including coalescence. It is important to mention that some other diffusion reaction models were already considered before [11–14].

2. $A + A \to A(0)$ anomalous coalescence through Thompson's method

An effective action to describe $A+A \to A(0)(k=2)$ reaction with Brownian diffusion condition was proposed by the present author [15,16], namely

$$A = \int_{l^d} \mathrm{d}^{\mathrm{d}} r \left[\frac{1}{2} D(\nabla n)^2 - hn + \frac{1}{3} K n^3 + \frac{1}{2} \frac{\partial (n^2)}{\partial t} \right] , \tag{2}$$

where n is a concentration and K a reaction rate. k represents the number of particles which coalesce. In the particular case (2) above, we have $k=2$ (see Ref. [10]). h and D are constants associated with source and diffusion of species, respectively.

By imposing $\delta A = 0$ for a constant t in (2), Nassif and Silva [2] obtained the following diffusion differential equation:

$$\frac{\partial n(r,t)}{\partial t} = D\nabla^2 n + h\delta(r) - Kn^2 , \tag{3}$$

where $h\delta(r)$ is a source term proposed by Krug [17], Kn^2 being the reaction term.

More recently, the present authors [10] obtained the following diffusion equation for $A + A \to A(0)$ reactions with anomalous diffusion condition (γ):

$$\frac{\partial n(r,t)}{\partial t} = D\nabla^{\gamma} n + h\delta(r) - Kn^2 . \tag{4}$$

The equation above is a fractional differential equation ($k = 2$) [10,18]. For $\gamma = 2$, we recover Eq. (3) for Brownian diffusion condition.

From (4), we have the effective action

$$A_{\gamma} = \int_{l^d} \mathrm{d}^{\mathrm{d}} r \left[\frac{1}{2} D(\nabla^{\gamma/2} n)^2 - hn + \frac{1}{3} K n^3 + \frac{1}{2} \frac{\partial (n^2)}{\partial t} \right] . \tag{5}$$

If $\gamma < 2$, we have superdiffusion. If $\gamma > 2$, we have subdiffusion.

In order to treat (5), we proceed in an analogous way to Thompson's reasoning [2] (see also Ref. [16]), which states the following scaling assumption for each term of the action above. First term:

$$\left| \int_{l^d} \mathrm{d}^{\mathrm{d}} r \left[\frac{1}{2} D(\nabla^{\gamma/2} n)^2 \right] \right| \sim l^{d-\gamma} \langle n^2 \rangle \sim 1 , \tag{6}$$

so that the mean squared value of n ($\langle n^2 \rangle$) behaves as

$$\langle n^2 \rangle \sim l^{\gamma - d} . \tag{7}$$

For the fourth term in (5), we have

$$\left| \int_{l^d} \mathrm{d}^{\mathrm{d}} r \left[\frac{1}{2} \frac{\partial (n^2)}{\partial t} \right] \right| \sim \langle \Omega \rangle \langle n^2 \rangle l^d \sim 1 , \tag{8}$$

where we have considered that

$$n(t) = n_0 \exp(-\Omega t) . \tag{9}$$

By introducing (7) into (8), we obtain

$$\langle \Omega \rangle^{-1} \equiv \tau \sim l^{\gamma} . \tag{10}$$

We observe that (10) points out to the signature of the non-Brownian character of these diffusion limited reactions [9,10]. Actually when we consider $\gamma < 2$ in (10), we have conditions beyond Brownian motion, which correspond to superdiffusion conditions.

For the second term in (5) we have

$$\left| -\int_{l^d} \mathrm{d}^{\mathrm{d}} r(hn) \right| \sim \langle h \rangle \langle n \rangle l^d \sim 1 . \tag{11}$$

Making $\langle h \rangle \sim 1$, from (11) and (10), we obtain the following scaling behavior:

$$\langle n \rangle \sim l^{-d} \sim \tau^{-(d/\gamma)} . \tag{12}$$

For the third term in (5), with the plausible hypothesis $\langle n^3 \rangle \sim \langle n^2 \rangle \langle n \rangle$ [8–10,15,16], and by using (12) above, we obtain

$$\langle K \rangle \sim l^{d-\gamma} \sim (l^{\gamma})^{d/\gamma - 1} \sim \tau^{d/\gamma - 1} \sim \tau^{d/d_c - 1} , \tag{13}$$

where

$$d_c = \gamma , \tag{14}$$

for $k = 2$ (see Ref. [10]).

3. An interpretation for anomalous coalescence of bubbles and droplets in 1d

Let us take n, the density of particles A, to represent bubble (or domain) concentration [1] which behaves like $n \sim t^{-d/\gamma}$, according to (12). It is customary to consider γ as a free parameter, where $\gamma < 2$ ($\gamma > 2$) is used to describe superdiffusion (subdiffusion) conditions and $\gamma = 2$ to designate the more usual Brownian diffusion. However, we can assume, for instance, γ to be a function of the dimensionality (d). As it is the case of the coalescence phenomena treated by JR, the concentration behavior (number of bubbles per volume) for $d \geqslant 2$ is $n(t) \sim t^{-1}$, which corresponds to a mean field regime. But, for $d \leqslant 2$, in particular for $d = 1$, they found an anomalous behavior, namely $n \sim t^{-1/4}$. So, in order to explain JR's numerical analysis, we have to take into account Eq. (14) by considering $\gamma = \gamma(d)$ through the following ansatz, where γ depends on the dimensionality:

$$\gamma = \gamma(d) = \begin{cases} 2, & d \geqslant d_c , \\ \dfrac{a}{d}, & d \leqslant d_c . \end{cases} \tag{15}$$

If we make $d_c = 2$, according to JR's result, and according to $A + A \to A$ coalescence model, then we have $\gamma(d_c) = d_c = 2 = a/2 \Leftrightarrow a = 4$. So we write

$$\gamma = \gamma(d) = \begin{cases} 2, & d \geqslant 2 \,, \\ \dfrac{4}{d}, & d \leqslant 2 \,, \end{cases} \tag{16}$$

in such a way that we have in fact $d_c = 2$ (upper critical dimension). Indeed this happens because, due to the condition (16) and also to the relation (14), we get the following consistency relation:

$$d_c = \gamma(d_c) = \frac{4}{d_c} \Leftrightarrow d_c = 2 \,. \tag{17}$$

Thus, for $d = d_c = 2$, we have $\gamma = 2$ (Brownian diffusion condition), and for $d = 1$ we have $\gamma = 4$ (a kind of subdiffusion condition). Starting from the condition for $d = 1$, here we want to show that the *ansatz* proposed by relation (16) leads to a kind of anomalous diffusion behavior for $d < 2$, such that we will be able to explain the "lack of theoretical explanation" mentioned by JR, for the case $d = 1$. In order to do that, we consider two basic assumptions. The first one is that the center of mass of the bubble coalesces through an anomalous diffusion process characterized by a certain diffusion length. The second one is that, simultaneously, each bubble increases its radius, being constrained by the conservation of its mass. Thus below the critical dimension ($d_c = 2$), we can write:

$$l \sim R \,, \tag{18}$$

where R is the radius of the bubble, and l the diffusion length.

The assumption above will be better justified firstly taking into account a conservation law for bubbles mass, which states that $nR^d \sim 1$ (constant), where n represents a homogeneous density of bubbles and R^d its volume. When n decreases, then R increases such that $n \sim R^{-d}$, taking into account a mean radius value $R(t)$ which increases in time. Now we can observe that this scaling law for the radius of the bubble is similar to the scaling obtained before by Thompson's approach ($nl^d \sim 1$) (Eq. (12)). However it must be stressed that the similarity between these two scaling relations will be restricted to dimensions below the upper critical dimension ($d < d_c = 2$). This is the main point to be understood.

In other words, we want to point out the fact that the particle A has an internal structure $R(t)$, namely an internal degree of freedom, which just scales like l, only for $d \leqslant 2$. That is because when we consider lower dimensionalities ($d \leqslant 2$), as for instance $d = 1$, the radius of each bubble increases fast enough to fill the empty space l that exists between the centers of mass of its nearest neighbors. Indeed, based on ansatz (16), we obtain $\gamma = 4$ for $d = 1$, which really represents a subdiffusion condition, i.e., $\gamma > 2$ [10].

On the other hand, for $d \geqslant 2$ (mean field regime), according to ansatz (16), the Brownian diffusion plays its role in such a way that the scale l increases faster than the radius R of the bubble, so that we have the following scaling law: $nl^2 \sim 1$, being $l \sim t^{1/2}$. In this condition we get $l \gg R$, and thus bubbles could pratically be seen as point particles A when they are compared with the length scale l of the diffusion process.

Therefore, since this corresponds to an expected behavior for point-like bubbles, we can understand why, only at $d=1$, an anomalous behavior was detected by JR numerical analysis.

Substituting (16) into (12), we finally obtain

$$n(t) \sim \begin{cases} t^{-1}, & d \geqslant d_c = 2 \text{ (mean field condition)} , \\ t^{-(d^2/4)}, & d \leqslant d_c = 2 . \end{cases} \tag{19}$$

If we make $d=1$ in (19), we finally obtain $n(t) \sim t^{-1/4}$. This is just the anomalous result [1], lacking a satisfatory explanation according to JR.

According to (10), we have $l \sim t^{1/\gamma}$; then by introducing (16) into this scaling relation (10), we obtain the following scaling relation for $l(t)$:

$$l = l(t) \sim \begin{cases} t^{1/2}, & d \geqslant 2 , \\ R(t) \sim t^{d/4}, & d \leqslant 2 . \end{cases} \tag{20}$$

We already know that $l(t)$ can be thought of as the radius of the bubble, only for $d \leqslant 2$, that is, $l(t) \sim R(t) \sim t^{d/4}$. On the other hand, for $d \geqslant 2$, we have $l \sim t^{1/2}$ and $R \sim t^{1/d}$. This means that, above two dimensions, we have different scalings for the diffusion length l, and the bubble radius R. Finally, based on relation (20) above, we verify that, for $d=1$, we have $R \sim t^{1/4}$, which corresponds to the anomalous result found in JR's numerical work [1].

4. An equivalent interpretation for JR results by using a diffusion constant depending on concentration of bubbles

Let us consider a diffusion constant $D = D_0 \langle n \rangle^{\alpha}$ to be put into an effective action A_α in order to replace the description provided by the exponent γ. Actually these two descriptions must be equivalent, giving the same behavior for $n(t)$ and $l(t)$. So we can write the following equivalent action to replace the first one (action (5)):

$$A_\alpha = \int_{l^d} \mathrm{d}^d r \left[\frac{1}{2} D_0 \langle n \rangle^{\alpha} (\nabla n)^2 - hn + \frac{1}{3} K n^3 + \frac{1}{2} \frac{\partial (n^2)}{\partial t} \right] , \tag{21}$$

D_0 is a constant. In (21), $\langle n \rangle$ means average concentration on the scale l.

From the first term of (21), we get the following scaling relation:

$$\langle n \rangle^{\alpha} \langle n^2 \rangle l^{d-2} \sim 1 . \tag{22}$$

For the fourth term we obtain

$$\frac{\langle n^2 \rangle l^d}{\tau} \sim 1 . \tag{23}$$

From the second term we get

$$\langle n \rangle l^d \sim 1 \Rightarrow l \sim \langle n \rangle^{-1/d} . \tag{24}$$

By comparing (22) with (23), being $\tau \sim l^{\gamma}$, we obtain

$$\langle n \rangle^{\alpha} \sim l^{2-\gamma} \Rightarrow l \sim \langle n \rangle^{\alpha/(2-\gamma)} . \tag{25}$$

For $\gamma = 2$ we have $\alpha = 0$ (mean field regime).

By comparing (25) with (24), we obtain the following relation by the equality of their exponents

$$\alpha = \left(\frac{\gamma - 2}{d}\right) . \tag{26}$$

Finally, by introducing the ansatz (16) for $\gamma(d)$ into (26), we get

$$\alpha = \begin{cases} \dfrac{2(2-d)}{d^2}, & d \leqslant 2 , \\ 0, & d \geqslant 2 . \end{cases} \tag{27}$$

For $d = 1$, we have $\alpha = 2$, leading to $D = D_0 \langle n \rangle^2$. This corresponds to an equivalent explanation for the anomalous coalescence condition found by JR.

For $d \geqslant 2$, $\alpha = 0 \Rightarrow D = D_0$ (constant), which represents the mean field regime with Brownian diffusion condition. It is worth stressing that below the critical dimension, for instance, in $d = 1$ $(D = D_0 \langle n \rangle^2)$, the effective diffusion coefficient depends on the density of bubbles. We interpret this fact as follows: for higher densities, the bubbles are squeezing each other and in this way, enhancing the diffusion; for lower densities, this process is attenuated, leading to a weakening of the diffusion rate.

According to (26), we have $\gamma = 2 + \alpha d$. Thus, by introducing this relation into (12) to replace γ, we can also write an equivalent scaling relation for the concentration, namely:

$$n \sim t^{-d/(2+\alpha d)} . \tag{28}$$

According to (27), if $\alpha = 2$, we have $d = 1$. Therefore, by putting these two results into the scaling (28) above, we simply verify by consistency, that $n \sim t^{-1/4}$. This is in agreement again with the JR's result. Indeed we have an equivalent description for anomalous coalescence of bubbles by using a diffusion constant, which depends on the concentration (n).

Now by putting (28) into (24), we obtain

$$l(t) \sim t^{1/(2+d\alpha)} . \tag{29}$$

Making $\alpha = 2(d = 1)$ in (29) above, we also recover the scaling relation obtained for the bubble growth as in JR's result, that is

$$l(t) \sim R(t) \sim t^{1/4} . \tag{30}$$

For $\alpha = 0$, $(d \geqslant 2)$, we recover the Brownian scaling condition $l(t) \sim t^{1/2}$.

5. Conclusions and prospects

In this paper, we have used Thompson's approach in order to interpret the anomalous coalescence of domains (bubbles) found by Josserand and Rica [1] in their numerical treatment of the NLSE by the addition of a quintic term. By proposing an explicit dependence on the dimensionality (d) for the parameter of anomalous diffusion (γ), we were able to show that this anomaly is restricted to dimensions smaller than two. So below two dimensions, both the radius of the bubble and the diffusion length are scaled in the same way. Above two dimensions, Brownian diffusion condition is recovered. So the bubble radius and the diffusion length are scaled in different ways with respect to time.

Alternatively, it was possible to describe the anomalous behavior of the bubbles by considering a diffusion equation where the diffusion coefficient depends on the density of bubbles.

Finally, a refinement of the numerical results of JR [1], just at $d_c = 2$, could lead to a logarithmic correction for the growth of the bubble radius, as always happens at the upper critical dimensions of the various kind of diffusion-controlled reactions [8,10,15,16].

In another paper, we extend the method applied here to study scalar field theories [19]. We also treat field theories described by Grassmann fields [20]. Our purpose in the latter was to work out, for instance, the QED_4 running coupling constant dependence on the energy scale.

Finally, Thompson's method, which was applied to various kinds of reactions limited by diffusion [8,10,15,16] 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 successfully employed in this task as an alternative way to the RG formalism.

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