Application of the Bogolyubov’s theory of weakly non-ideal Bose gas on the A+A, A+B, B+B reaction-diffusion system

Zoran Konkoli

Department of Applied Physics
Chalmers University of Technology
and Göteborg University,
SE 412 96 Göteborg,
Sweden

(March 22, 2022)

Theoretical methods for dealing with diffusion-controlled reactions inevitably rely on some kind of approximation and to find the one that works on a particular problem is not always easy. In here the approximation used by Bogolyubov to study weakly non-ideal Bose gas, to be referred to as weakly non-ideal Bose gas approximation (WBGA), is applied in the analysis of of the three reaction-diffusion models (i) \( A + A \rightarrow \emptyset \), (ii) \( A + B \rightarrow \emptyset \) and (iii) \( A + A, B + B, A + B \rightarrow \emptyset \) (the ABBA model). The two types of WBGA are considered, the simpler WBGA-I and more complicated WBGA-II. All models are defined on the lattice to facilitate comparison with computer experiment (simulation). It is found that the WBGA describe A+B reaction well, it reproduces correct \( d/4 \) density decay exponent. However, it fails in the case of the A+A reaction and the ABBA model. (To cure deficiency of WBGA in dealing with A+A model the hybrid of WBGA and Kirkwood superposition approximation is suggested.) It is shown that the WBGA-I is identical to the dressed tree calculation suggested by Lee in J. Phys. A 27, 2633 (1994), and that the dressed tree calculation does not lead to the \( d/2 \) density decay exponent when applied to the A+A reaction, as normally believed, but it predicts \( d/4 \) decay exponent. Last, the usage of the small \( n_0 \) approximation suggested by Mattis and Glasser in Rev. Mod. Phys. 70(3), 979 (1998) is questioned if used beyond A+B reaction-diffusion model.

I. INTRODUCTION

A variety of methods have been used to study diffusion-controlled reactions (see, e.g., refs. [1–8] for review) ranging from simplest pair-like or Smoluchowskii approach \([9]\) towards more sophisticated methods such as many particle density function formalism \([4,5]\) and field theory \([6–8]\). In here, we focus on the field theory approach which is exact but, like in any other theory, one needs approximations to solve the problem. The particular way of making approximate calculations will be analyzed, the Bogolyubov’s theory of weakly non-ideal Bose gas \([10]\), to be referred to in the following as Weakly non-ideal Bose Gas Approximation (WBGA).

The field theory is very attractive since it offers systematic way to do calculation and there are well known procedures how to represent stochastic dynamics of reaction-diffusion systems as field theory. Such mapping can be carried out for lattice- and off-lattice models, see \([6]\) and \([9]\) respectively for description. Final result is that the dynamics is governed by a second quantized Hamiltonian \( H(a, a^\dagger) \),

\[
\frac{\partial}{\partial t} \Psi(t) = -H(a, a^\dagger) \Psi(t)
\]  

and system configuration at time \( t \) can be extracted from state vector \( \Psi(t) \). All observables can be expressed as a field theoretic averages over products of creation and annihilation operators \( a^\dagger \) and \( a \).

There is no need whatsoever to resort to the use of field theory as all calculations could be done without it. The reasons for using it are mostly practical. Field theory is a powerful book-keeping device. First, approximations involved can be made more transparent and, second, due to this transparency it is relatively straightforward to borrow approximations from other problems (and related forms of field theory).

However, despite its elegance, when applied to the reaction-diffusion systems, field theory seems to work with limited success. Most often the only practical procedure of solving field theory is perturbative calculation. Diffusion is set up as the zeroth order problem and reaction is perturbation. Problem is that in the most interesting regime, when dimension of the system is low (below some critical dimension), perturbation series diverges due to infra-red divergences. Any non-field theoretic approach which aims at perturbative treatment will suffer in a similar way.

The infra-red divergences are normally controlled in the framework of the renormalization group (RG) tech-
The WBGA was used to study reaction-diffusion systems previously [8,9,11–13]. In somewhat technical terms, the basic idea behind WBGA is to neglect the products containing three or higher number of annihilation operators having non-zero wave vector in the Hamiltonian. This procedure leads to closed set of equations for particle density and correlation functions. Solving these equations amounts to resummation of infinite series of diagrams. In this way WBGA appears as a non-perturbative technique which can be used to control infra-red divergences of perturbation series. In the following, we will distinguish between two types of approximations to be refereed to as WBGA-I or WBGA-II which result in linear or nonlinear set of equations of motion respectively.

On the more intuitive basis, the neglect of fluctuations on the shorter length scale (large \( k \) vectors) has to do with the slowness of diffusion. For initial conditions when particle density is uniform there is no \( k \neq 0 \) component in average particle density and the density profile is flat. Since diffusion is a very slow process one expects that this profile is kept all the time up to a small perturbation. This picture is likely to be true when particle density is low when compared to the reaction range, which is summarized in the condition that \( nr^d \ll 1 \) where \( n \) and \( r \) denote the particle density and the reaction range [9]. Naturally, there are other scales in the problem (which change in time) and this kind of thinking can not be employed without encountering problems [4]. In reality, one really has to test the WBGA on the particular model to see whether it works.

To analyze properties of the WBGA method, we apply it in the analysis of three diffusion-controlled reactions (i) the A+A, (ii) the A+B and (iii) the ABBA model. The ABBA model includes A+A, A+B and B+B reactions simultaneously which allows for competitions between A+A and A+B reactions (see ref. [14,15] for more details). The A+A and A+B models have been studied by variety of methods (see, e.g., ref. [16] for review). In here, the focus is on the WBGA studies. Apart from few initial studies of the A+A and A+B models the WBGA have not been widely used. These early applications of WBGA on A+A and A+B reaction-diffusion systems are mostly done for stationary situation (and decay from it) and are listed in refs. [11] (A+A) and [12,13] (A+B). Also, the WBGA reappears in paper [6] where it is used to study the A+B reaction.

The purpose of this work is twofold. First, we study A+A and A+B reactions with uncorrelated initial conditions with particles Poisson-distributed [17] at initial time \( t = 0 \). In previous work which employed WBGA method in refs. [11–13] it was assumed that particles are initially correlated, with a initial condition being prepared in a somewhat special way [18]. Second, once the workings of the WBGA approximation is illuminated, we apply the WBGA method to analyze the more complicated ABBA model. This model was studied previously with field theoretic RG technique using \( e \)-expansion and numerical simulation [14,15]. The ABBA model describes a mixture of the A+A and A+B reactions which occur at the same time. The A+A (A+B) component bias kinetics towards \( d/2 \) (\( d/4 \)) decay exponent and it is not a priori clear which exponent will prevail. The analysis in [14,15] shows that both A and B particles decay with \( d/2 \) decay exponent and different amplitudes.

The A+A model has been studied by variety of methods and lot is know about it’s behavior. The study most relevant for this work is given in ref. [19]. For uncorrelated initial conditions particle density \( n \) decays asymptotically as \( n \sim A(Dt)^{-d/2} \) for \( d < 2 \) while there is logarithmic correction at \( d = 2 \) as \( n \sim \ln(Dt)/(8\pi D t) \), where \( d \) denotes dimension of system, \( t \) is time and \( D \) denotes diffusion constant. Amplitude \( A \) is universal number independent on the details of the model. Also, the exact solution of the model is possible at \( d = 1 \) where \( n \sim 1/\sqrt{8\pi Dt} \) [20].

The \( d/2 \) decay exponent of the A+A reaction is robust in a sense that even simplest pair like approach (e.g. Smoluchowski) predicts this exponent. Thus, it is natural to test WBGA on the A+A model. It will be shown that, somewhat surprisingly, WBGA fails to describe A+A reaction: WBGA-I predicts \( d/4 \) decay exponent while WBGA-II gives mean field exponent.

Taking slightly more complicated reaction scheme, such as the A+B, leads to very hard problem where calculation methods start to differ in their predictions. The nature of the asymptotics of A+B reaction when initial number of A and B particles is equal has been hotly debated for decades. For example, Smoluchowski approach predicts \( d/2 \) decay exponent [4,5,9]. Field theoretic RG method predicts correct \( d/4 \) decay for \( 3 < d < 4 \) [21], while for other dimensions nothing can be said in the RG framework. Strangely enough, seemingly the most sophisticated coupled-cluster technique argues for mean field exponent [22]. The true decay is governed by \( d/4 \) exponent as shown by work of Bramson and Lebowitz which provided strict mathematical proof [23]. It will be shown that when particles are initially uncorrelated, i.e. Poisson-distributed, both the WBGA-I and WBGA-II predict \( d/4 \) decay exponent. Strangely enough, WBGA fails on simpler A+A reaction while it describes properly more complicated A+B reaction.

The paper is organized as follows. In section II the
model to be studied is specified in detail, and mapping to the field theory is described. The outcome of this section is Hamiltonian which describes the most general two species reaction-diffusion model. In section III equations of motion for density and correlation functions are derived using WBGA method. In section IV the WBGA approach is used to describe A+A model, with application of WBGA-I discussed in section IV A, and application of WBGA-II in section IV B. Also in section IV A equivalence of dressed tree calculation with WBGA-I is shown. Section IV C discusses modification of Kirkwood superposition approximation in the spirit of WBGA. In section V A+B model is studied by using WBGA-I and WBGA-II methods. Finally, the analysis of the most complicated of three models studied here, the ABBA model, is presented in section VI. Workings of WBGA-I are analyzed in section VIA and of WBGA-II in section VIB. The step by step merger of WBGA and Kirkwood superposition approximation is discussed in VlC. The summary and outline of future work is given in section VII.

II. THE MODEL AND THE MAPPING TO THE FIELD THEORY

The mapping to the field theory will be carried out for the most general two-species reaction-diffusion model. The A+A, A+B and the ABBA model will be obtained as special cases. It will be assumed that particles can not be created, neither by external source, nor by birth process. In the most general version of the two species reaction-diffusion model each of the A or B particles jumps onto the one of the neighboring lattice sites with rate (or diffusion constant) \( D_A \) or \( D_B \), irrespectively of occupation number of the site where particle jumps to. Apart from diffusing particles annihilate in pairs. Particle \( \rho \) sitting at lattice site \( x \) and particle \( \nu \) sitting at the site \( y \) are assumed to annihilate with rate \( \sigma_{xy}^{\text{ann}} \). This is schematically denoted as

\[
\rho(x) + \nu(y) \rightarrow 0
\]  

where \( \rho, \nu = A, B \) and \( x, y = 1, 2, 3, \ldots, V \). It is assumed that there are \( L \) lattice sites in one direction, and for \( d \) dimensions total number of sites equals \( V = L^d \). Labels \( x \) and \( y \) denote lattice sites.

The stochastic dynamics of the most general two-species model is governed by the master equation of the system. The master equation describes transitions between different configurations \( c \). The configuration of the system is specified by the occupancy of lattice sites at certain time \( t \);

\[
c = (n_1, m_1, \ldots, n_x, m_x, \ldots, n_y, m_y, \ldots, n_V, m_V) \]  

\( n_x \) and \( m_x \) count number of A and B particles respectively at \( x \)-th lattice site; \( n_x, m_x = 0, 1, 2, \ldots \) and \( x = 1, 2, \ldots, V \). The quantity of interest is \( P(c; t) \), which denotes probability that at given time \( t \) system is in the configuration \( c \).

Diffusion and reaction contribute independently to change of \( P(c; t) \):

\[
\frac{\partial}{\partial t} P(c; t) = \dot{P}_D(c; t) + \dot{P}_R(c; t)
\]  

The influence of diffusion is described by

\[
\dot{P}_D(c; t) = \sum_{x; e(x)} \left( D_A [(n_i + 1)P(n_x + 1, n_e - 1; t) - n_i P(c; t)] + D_B [(m_i + 1) \times P(m_x + 1, m_e - 1; t) - m_i P(c; t)] \right)
\]  

where notation \( P(\ldots; t) \) indicates that content of the sites specified by \( \ldots \) has been modified in \( t \). The \( \sum_{x; e(x)} \) denotes sum over all first-neighbor sites of the site \( x \). The change of \( P(c; t) \) driven by reactions is given by

\[
\dot{P}_R(c; t) = \sum_x \sigma_{xx}^{AA} \frac{(n_x + 2)(n_x + 1)}{2} P(n_x + 2; t)
\]  

\[
+ \sum_x \sigma_{xx}^{BB} \frac{(m_x + 2)(m_x + 1)}{2} P(m_x + 2; t)
\]  

\[
+ \sum_x \sigma_{xx}^{AB} (n_x + 1)(m_x + 1) P(n_x + 1, m_x + 1; t)
\]  

\[
+ \sum_{x > y} \sigma_{xy}^{AA} (n_x + 1)(n_y + 1) P(n_x + 1, n_y + 1; t)
\]  

\[
+ \sum_{x > y} \sigma_{xy}^{BB} (m_x + 1)(m_y + 1) P(m_x + 1, m_y + 1; t)
\]  

\[
+ \sum_{x \neq y} \sigma_{xy}^{AB} (n_x + 1)(m_y + 1) P(n_x + 1, m_y + 1; t)
\]  

\[
- \left[ \sum_x \sigma_{xx}^{AA} \frac{n_x(n_x - 1)}{2} + \sum_x \sigma_{xx}^{BB} \frac{m_x(m_x - 1)}{2} \right]
\]  

\[
+ \sum_x \sigma_{xx}^{AB} n_x m_x + \sum_{x > y} \sigma_{xy}^{AA} n_x n_y
\]  

\[
+ \sum_{x > y} \sigma_{xy}^{BB} m_x m_y + \sum_{x \neq y} \sigma_{xy}^{AB} n_x m_y \right] P(c; t)
\]  

The form of the master equation describing reactions can not be made more compact since distinction has to be made between reaction on the same and different lattice sites. For example, the term describing A+A reaction at the same lattice site has the pre-factor \( n_x(n_x - 1) \) while for two different sites another form \( n_x n_y \) has to be used.

The master equation (4) is the first order differential equation and one has to specify initial condition in the form \( P(c; 0) \) for all \( c \). In the following it will be assumed that \( P(c; 0) \) is Poisson distribution with averages denoted
by \( n_{0,A} \) and \( n_{0,B} \) for \( A \) and \( B \) particles respectively. This means that \( P(c;0) \) factorises,

\[
P(c;0) = \Pi_{x=0,1,2,...,V} p(n_x, n_{0,A}) p(m_x, n_{0,B})
\]

(7)

where \( p(n, \tilde{n}) \) denotes Poisson distribution function

\[
p(n, \tilde{n}) = e^{-\tilde{n}} n^n / n!
\]

(8)

In general, form of \( \Psi_0 \) depends on the initial particle distribution and for Poisson-distributed particles equals \( \Psi_0 = \exp \left[ n_{0,A} \sum_x (a_x \dagger - 1) + n_{0,B} \sum_x (b_x \dagger - 1) \right] |0\rangle \)

(14)

Since \( \Psi(t) \) is available (at least in principle) one can calculate various observables with following recipe

\[
\langle O(n_x(t)) \rangle = \langle 1|O(a_x \dagger a_x)|\Psi(t)\rangle
\]

(15)

where \( O(n_x) \) denotes any function which depends on particle numbers in arbitrary Way. The generalization of Eq. (15) for more complicated form for \( O(n_x, m_y, ...) \) is trivial. Vector \langle 1 \rangle \) is given by

\[
\langle 1 \rangle \equiv \langle 0| \exp \left[ \sum_x (a_x + b_x) \right]
\]

(16)

being left eigenvector of \( a_x \dagger \) and \( b_x \dagger \) with eigenvalue 1. To see that Eq. (15) indeed evaluates observables correctly one can expand function \( O \) in Taylor series in \( n_x \) and check that for every term in Taylor series Eq. (15) works.

Following ref. [6], since \langle 1|a_x \dagger \neq 0 \), it is useful to transform Eq. (15) slightly in order to obtain form where \langle 1 \rangle changes into the vacuum state \langle 0 \rangle. This makes calculation somewhat easier since one can use property of the vacuum that \langle 0|a_x \dagger = 0 \). To do the transformation following identity proves useful,

\[
\langle 1|O(a_x, a_x)|0\rangle = \langle 0|O(a_x + 1, a_x)|0\rangle
\]

(17)

and by using (17) Eq. (15) can be written in the form

\[
\langle O(n_x(t)) \rangle = \langle 0|O((a_x + 1)a_x)e^{-Ht}|\Psi_0\rangle
\]

(18)

where bar over \( H \) and \( \Psi_0 \) indicates that substitution

\[
a_x \dagger \rightarrow a_x \dagger + 1 \quad , \quad b_x \dagger \rightarrow b_x \dagger + 1 \quad , \quad x = 0, 1, 2, ..., V
\]

(19)

have been made. The \( \Psi_0 \) is given by

\[
\Psi_0 = \exp \left[ n_{0,A} \sum_x a_x \dagger + n_{0,B} \sum_x b_x \dagger \right] |0\rangle
\]

(20)

and \( \bar{H} = \bar{H}_D + \bar{H}_R \). After the shift \( \bar{H}_D \) does not change the form, i.e. \( \bar{H}_D = \bar{H}_D \), while \( \bar{H}_R \) changes into

\[
\bar{H}_R = \frac{1}{2} \sum_{x,y} \sigma_{xy}^{AA} (a_x \dagger a_y + a_x a_y) b_x a_y +
\]

\[
+ \frac{1}{2} \sum_{x,y} \sigma_{xy}^{BB} (b_x \dagger b_y + b_x b_y) b_x b_y +
\]

\[
+ \sum_{x,y} \sigma_{xy}^{AB} (a_x \dagger b_y + a_x b_y) a_x b_y
\]

(21)

In the following we compactify notation and use
\[ \langle f(a_x, a_y, \ldots) \rangle \equiv \langle 0|f(a_x, a_y^\dagger, \ldots) e^{-\hat{H}t}|\bar{\Psi}_0 \rangle \quad (22) \]

where \( f \) denotes any function of operators \( a_x, a_y^\dagger, b_x \) and \( b_y^\dagger \) for any \( x \) and \( y \). Also notation
\[ \bar{\Psi}(t) \equiv e^{-\hat{H}t}|\bar{\Psi}_0 \rangle \quad (23) \]

will be useful.

To avoid effects of boundaries periodic boundary conditions are assumed and one can introduce Fourier transforms for operators,
\[ a_x = \frac{1}{\sqrt{V}} \sum_k e^{ikx} a_k, \quad a_x^\dagger = \frac{1}{\sqrt{V}} \sum_k e^{-ikx} a_k^\dagger \quad (24) \]
\[ b_x = \frac{1}{\sqrt{V}} \sum_k e^{ikx} b_k, \quad b_x^\dagger = \frac{1}{\sqrt{V}} \sum_k e^{-ikx} b_k^\dagger \quad (25) \]

and reaction rates
\[ \sigma^\rho_\nu = \frac{1}{V} \sum_k \sigma^\rho_\nu e^{-ikx}, \quad \sigma^\rho_\nu = \sum_x \theta^\rho_\nu e^{-ikx} \quad (26) \]

with \( \rho, \nu = A, B \). For convenience, Fourier transforms are defined slightly differently for operators and reaction rates (just to reduce explicit occurrence of \( V \) in expressions later on). Also, it is useful to express Hamiltonian \( \hat{H} \) in terms of creation and annihilation operators in \( k \)-space. Starting from (11) and (21), and using (24)-(26) gives
\[ H_D = D_A \sum_k k^2 a_k^\dagger a_k + D_B \sum_k k^2 b_k^\dagger b_k + \mathcal{O}(k^4) \quad (27) \]

and
\[ \hat{H}_R = \frac{1}{\sqrt{V}} \sum_{q,k} \sigma^A A_{kq}^\dagger a_k q a_q + \frac{1}{2V} \sum_{q,k,l} \sigma^A A_{kq}^\dagger a_k q a_l + \sigma^A A_{kq} a_k q a_l^\dagger \\
+ \frac{1}{2V} \sum_{q,k,l} \sigma^B B_{kq}^\dagger b_k q b_l + \frac{1}{2V} \sum_{q,k,l} \sigma^B B_{kq} b_k q b_l^\dagger \\
+ \frac{1}{V} \sum_{q,k,l} \sigma^A B_{kq}^\dagger (a_k q b_l + b_k q a_l^\dagger) + \frac{1}{V} \sum_{q,k,l} \sigma^A B_{kq} a_k q b_l^\dagger + \sigma^B b_k q a_l^\dagger \\
+ \frac{1}{V} \sum_{q,k,l} \sigma^B B_{kq} a_k q b_l + \sigma^B a_k q b_l^\dagger \quad (28) \]

III. EQUATIONS OF MOTION FOR DENSITY AND THE CORRELATION FUNCTIONS

Equation (18) summarizes how observables are calculated within the field theory formalism. We continue with the specific case of local particle densities \( n_A(x,t) \) and \( n_B(x,t) \), which can be calculated with \( O = a_k^\dagger a_k \) and \( O = b_k^\dagger b_k \) respectively; using (18) one gets \( n_A(x,t) = \langle a_x \rangle \) and \( n_B(x,t) = \langle b_x \rangle \), or more explicitly
\[ n_A(x,t) = \langle 0|a_x|\bar{\Psi}(t)\rangle = \langle 0|a_x e^{-\hat{H}t}|\bar{\Psi}_0 \rangle \quad (29) \]
\[ n_B(x,t) = \langle 0|b_x|\bar{\Psi}(t)\rangle = \langle 0|b_x e^{-\hat{H}t}|\bar{\Psi}_0 \rangle \quad (30) \]

If initial conditions are translationally invariant, which is the case for Poisson-distributed particles, local particle densities are position independent, i.e. \( n_A(x,t) = n_A(t) \) and \( n_B(x,t) = n_B(t) \). Also at \( t = 0 \) \( n_A(0) = n_{0A} \) with \( \rho = A,B \). It is convenient to re-express \( n_A(t) \) and \( n_B(t) \) as \( n_A(t) = \frac{1}{V} \sum_k n_A(x(t), t) \) and \( n_B(t) = \frac{1}{V} \sum_k n_B(x(t), t) \). Using field theory \( n_A(t) \) and \( n_B(t) \) can be calculated from
\[ n_A(t) = \frac{1}{V} \langle \sum_x a_x \rangle = \frac{1}{\sqrt{V}} \langle a_0 \rangle \quad (31) \]
\[ n_B(t) = \frac{1}{V} \langle \sum_x b_x \rangle = \frac{1}{\sqrt{V}} \langle b_0 \rangle \quad (32) \]

where the sum over \( x \) divided by \( \sqrt{V} \) was recognized as \( k = 0 \) component of \( a_k \) and \( b_k \).

The equations of motion for \( n_A(t) \) and \( n_B(t) \) can be derived as follows. \( n_A(t) \) and \( n_B(t) \) are proportional to \( \langle a_0 \rangle \) and \( \langle b_0 \rangle \) respectively, and it is sufficient to derive equations for them. Taking time derivative of \( \langle a_0 \rangle \) and \( \langle b_0 \rangle \) gives,
\[ \frac{\partial}{\partial t} \langle a_0 \rangle = -\langle [a_0, \hat{H}] \rangle \quad (33) \]
\[ \frac{\partial}{\partial t} \langle b_0 \rangle = -\langle [b_0, \hat{H}] \rangle \quad (34) \]

The commutator emerges when time derivative acts on \( \exp(-\hat{H}t) \) [24]. Evaluating the commutator with \( \hat{H} \) given in (27) and (28), and taking into account (31) and (32) gives
\[ \frac{\partial n_A}{\partial t} = -\left[ \sigma^A A_{kq} n_A + \frac{1}{V} \sum_{k \neq 0} \sigma^A A_{kq} \Gamma^A_k \right] + \frac{1}{\sqrt{V}} \sum_{k \neq 0} \left( \sigma^A A_{kq} \Gamma^A_k \right) \quad (35) \]
\[ \frac{\partial n_B}{\partial t} = -\left[ \sigma^B B_{kq} n_B + \frac{1}{V} \sum_{k \neq 0} \sigma^B B_{kq} \Gamma^B_k \right] + \frac{1}{\sqrt{V}} \sum_{k \neq 0} \left( \sigma^B B_{kq} \Gamma^B_k \right) \quad (36) \]
where
\[
\Gamma_k^{AA} = \langle a_k a_{-k} \rangle
\]  
(37)
\[
\Gamma_k^{BB} = \langle b_k b_{-k} \rangle
\]  
(38)
\[
\Gamma_k^{AB} = \langle a_k b_{-k} \rangle
\]  
(39)

To derive (35) and (36) the sum over \( k \) is split into \( k = 0 \) and \( k \neq 0 \) parts and assumption is made that \( k = 0 \) components are non-fluctuating, i.e. \( \langle a_0 a_0 \rangle \approx \langle a_0 \rangle \langle a_0 \rangle \) and likewise for \( \langle b_0 b_0 \rangle \) and \( \langle b_0 \rangle \). Evaluating commutators gives equations of motion,

\[
\frac{\partial}{\partial t} \Gamma_k^{AA} = -2D_{AB} k^2 \Gamma_k^{AA} - \left[ \sigma_k^{AA} n_A^2 + \frac{1}{V} \sum_{q \neq k} \sigma_{k-q}^{AA} \Gamma_{k-q}^{AA} + 2(\sigma_0^{AA} + \sigma_k^{AA}) n_A \Gamma_k^{AA} + \sigma_k^{AB} n_A (\Gamma_k^{AB} + \Gamma_k^{BA}) + 2 \sigma_0^{AB} n_B \Gamma_k^{AA} \right]
\]  
(40)

\[
\frac{\partial}{\partial t} \Gamma_k^{BB} = -2D_{BB} k^2 \Gamma_k^{BB} - \left[ \sigma_k^{BB} n_B^2 + \frac{1}{V} \sum_{q \neq k} \sigma_{k-q}^{BB} \Gamma_{k-q}^{BB} + 2(\sigma_0^{BB} + \sigma_k^{BB}) n_B \Gamma_k^{BB} + \sigma_k^{AB} n_B (\Gamma_k^{AB} + \Gamma_k^{BA}) + 2 \sigma_0^{AB} n_A \Gamma_k^{BB} \right]
\]  
(41)
\[
\frac{\partial}{\partial t} \Gamma_k^{AB} = -(D_A + D_B) k^2 \Gamma_k^{AB} - \left[ \sigma_k^{AB} n_A n_B + \frac{1}{V} \sum_{q \neq k} \sigma_{k-q}^{AB} \Gamma_{k-q}^{AB} - [(\sigma_0^{AA} + \sigma_0^{BB}) n_A + (\sigma_0^{BB} + \sigma_0^{AA}) n_B] \Gamma_k^{AB} - \sigma_k^{AB} n_A \Gamma_k^{BB} - n_B \Gamma_k^{AA} \right]
\]  
(42)

Eqs. (40), (41) and (42) are approximate since correlators of type \( \langle a_k a_q a_l \rangle \) with \( k \neq 0, q \neq 0, \) and \( l \neq 0 \) are assumed to be small. This is exactly the content of the WBGA.

Few comments about the inversion symmetry (in k-space) of \( \Gamma_{k, \rho, \mu}^{\rho, \sigma} \) for \( \rho = A, B \) are in order. By construction, \( \Gamma_{k, \rho, \mu}^{\rho, \sigma} = \Gamma_{-k, \rho, \mu}^{\rho, \sigma} \) for \( \rho = A, B \) since these functions represent correlations for same operator types. It is not obvious whether this property holds for \( \Gamma_k^{AB} \) which describes correlations for different operator types. Using Eq. (42) to derive equation of motion for \( \Gamma_k^{AB}(t) \equiv \Gamma_k^{AB}(t) - \Gamma_k^{BA}(t) \) one can see that \( \Gamma_k^{AB}(t) \) is solution provided \( \Gamma_k^{AB}(0) = 0 \). The initial conditions for \( \Gamma_k^{\rho, \sigma} \) with \( \rho, \sigma = A, B \) are given by

\[
\Gamma_k^{\rho, \sigma}(0) = \delta_{k,0} V n_{0, \rho} n_{0, \sigma}, \quad \rho, \sigma = A, B
\]  
(43)

where \( \delta_{x,y} \) denotes Kronecker delta-function, will be used. Thus \( \Gamma_k^{(-1)}(0) \) is indeed zero. It follows that \( \Gamma_k^{AB}(t) = \Gamma_k^{AB}(t) \) for every \( t \geq 0 \). In the following whenever \( \Gamma_k^{AB} + \Gamma_k^{BA} \) appears in the equations of motion, we will use assumption of inversion symmetry and shorten expression to \( 2\Gamma_k^{AB} \). Naturally, if this inversion symmetry is broken at \( t = 0 \) one has to keep full form \( \Gamma_k^{AB} \) in the equations of motion, but such case is not considered here.

The last terms in Eqs. (40)-(42), which are product of density and correlator, and appear to be third order in density \( O(n^3) \), lead to non-linear equations of motion. These terms come from averages of the type \( \langle a_k a_q a_l \rangle \) where one of \( \{k, q, l\} \) momenta is zero while remaining two are not. One example would be \( \langle a_k a_0 a_l \rangle \) which is approximatively equal to \( \langle a_0 a_l \rangle \). (Same discussion would apply irrespectively which operator one uses in average, \( a_k \) or \( b_k \).) Being third order in density, it is tempting to neglect these \( O(n^3) \) terms, since one expects that leading contribution should come from terms which are second order in density \( O(n^2) \), e.g. first and second terms on the right hand side of Eq. (40) and likewise for Eqs. (41) and (42). To test the effect of neglecting or keeping \( O(n^3) \) terms two approximations will be studied WBGA-I or WBGA-II with \( O(n^3) \) terms taken away or kept in the calculation. WBGA-I approximation results in a linear set of equations which makes the analytical analysis possible. Also, as formulated above, the WBGA-II and WBGA appear to be equivalent. In the following, the term WBGA will imply both WBGA-I and WBGA-II.

The equations of motion for the three models we wish to study, the A+A, A+B and ABBA are easily extracted from the most general form given in (35)-(36) and (40)-(42). To obtain equations of motion for the ABBA model one simply sets \( D_A = D_B = D \) and

\[
\sigma_{xy}^{AA} = \sigma_{xy}^{BB} = \lambda \delta_{x,y}, \quad \sigma_{xy}^{AB} = \delta \delta_{x,y}
\]  
(46)

An obvious distinction is being made between Kronecker delta-function \( \delta_{x,y} \) and the symbol \( \delta \) which denotes the reaction rate. Thus particles have to meet at the same lattice site in order to react. Further, to obtain the A+A model one simply sets \( \delta = 0 \) (this decouples A+A and B+B reactions, i.e. particles A and B move and react independently of each other). To get A+B model one takes \( \lambda = 0 \) which rules out the A+A reaction. In the following section we continue with analysis of the A+A model within WBGA framework.
IV. WBGA APPLIED TO THE A+A REACTION

Using (46) with $\delta = 0$ in (35)-(36) and (40)-(42) gives equation of motion for the density

$$\frac{\partial n}{\partial t} = -\lambda [n^2 + \Phi]$$

(47)

and the correlator

$$\frac{\partial}{\partial t} \Gamma_k = -2Dk^2 \Gamma_k - \lambda [n^2 + \Phi] - 4\lambda n \Gamma_k$$

(48)

Let $A$ has been dropped on $n_A$ and $\Gamma_k^A$ to simplify notation, and likewise $n_{0,A}$ is shortened to $n_0$. $\Phi(t)$ is implicitly defined by correlators,

$$\Phi(t) = \frac{1}{V} \sum_{k \neq 0} \Gamma_k(t)$$

(49)

Thus equations above are meant to describe the model where only one type of species, A, jumps on the lattice and particles have a chance to react only when at the same lattice site. The equations above will be solved in the following two subsections using WBGA-I and WBGA-II approaches.

A. The WBGA-I approximation

In the WBGA-I approximation, when term proportional to $n \Gamma_k$ is dropped, Eq. (48) can be studied analytically. Uncorrelated (Poisson-like) initial condition is described by $\Gamma_k = \delta_{k,0} V n_0^2$ and solution of (48), with $k \neq 0$, reads

$$\Gamma_k(t) = -\lambda \int_0^t dt' e^{-2Dk^2(t-t')} [n(t')^2 + \Phi(t')]$$

(50)

Please note that the $\Gamma_0(t)$ is determined from $\Gamma_0(t) = Vn(t)^2$ (thermodynamic limit) and not from (50). Summation of Eq. (50) over $k \neq 0$ and division by $V$ gives

$$\Phi(t) = -\lambda \int_0^t dt' G(t-t') [n(t')^2 + \Phi(t')]$$

(51)

where

$$G(t-t') \equiv \frac{1}{V} \sum_{k \neq 0} e^{-2k^2D(t-t')}$$

(52)

was introduced. As shown in the appendix A, for large lattice size when $V \to \infty$, expression above can be approximated as

$$G(t-t') \approx [8\pi D(t-t' + \eta)]^{-d/2}$$

(53)

where $\eta = \frac{1}{8\pi D}$.

Equations (47), (51) and (53) completely specify $n(t)$. It is not possible to solve them analytically, however, large time behavior of $n(t)$ can be extracted. To do this we introduce $\varphi \equiv n^2 + \Phi$ and rewrite Eqs. (47) and (51) as

$$\frac{\partial n}{\partial t} = -\lambda \varphi$$

(54)

$$\varphi(t) = n(t)^2 - \lambda \int_0^t dt' G(t-t') \varphi(t')$$

(55)

which completely specify $n(t)$.

By using Laplace transform it is possible to transform equations (54) and (55) into a single equation. Laplace transform is defined as

$$X(s) = \int_0^\infty dt e^{-st} \varphi(t)$$

(56)

For $X = n$, $\varphi$ same symbol will be used for Laplace transform as for the original function. The only exception to the rule are two cases. For $X(t) = n(t)^2$, $X(s) = n_2(s)$, while for $X(t) = G(t)$, $X(s) = g(s)$.

Taking Laplace transform of Eq. (55) one gets $\varphi(s) = n_2(s) - \lambda g(s) \varphi(s)$, and combining it with $\varphi(s) = (sn(s) - n_0) / \lambda$ from (54) gives

$$n_2(s) = \left[ g(s) + \frac{1}{X} \right] [n_0 - sn(s)]$$

(57)

The $g(s)$ is the Laplace transform of $G(t)$,

$$g(s) = (8\pi D)^{-d/2} e^{\eta s} s^{d/2-1} \Gamma(1-d/2, \eta s)$$

(58)

$\Gamma(\beta, x)$ denotes incomplete Gamma function;

$$\Gamma(\beta, x) = \int_x^\infty du u^{-1+\beta} e^{-u}$$

(59)

The analytic continuation of $\Gamma(\beta, x)$ is possible. For non-integer $\beta$ and $\beta = 0$, $\Gamma(\beta, z)$ is multiple-valued function of $z$ with a branch point at $z = 0$, and has no poles. Dividing by $g(s) + 1 / \lambda$ Eq. (57) results in

$$sn(s) - n_0 = -\lambda_{\text{eff}}(s)n_2(s)$$

(60)

where $\lambda_{\text{eff}}(s)$ denotes Laplace transform of the effective reaction rate,

$$\lambda_{\text{eff}}(s) = \frac{\lambda}{1 + \lambda g(s)}$$

(61)

Finally, taking inverse Laplace transform of (60) gives
\[ \frac{\partial n}{\partial t} = - \int_0^t dt' \lambda_{\text{eff}}(t - t') n(t')^2 \quad (62) \]

Equations (54)-(55) and Eq. (62) are fully equivalent. Both equations have been dealt with before, however, in a very different context. Eq. (62) was obtained in ref. [19] through a diagrammatic technique and referred to as the dressed-tree calculation. Thus in here we have shown that WBGA-I is equivalent to the dressed tree calculation. Eqs. (54)-(55) have been also obtained in the study of the entirely different A+B model in ref. [6].

Studies [19] and [6] suggest contradictory result: ref. [19] argues that the dressed tree calculation gives \( d/2 \) decay exponent for particle density, while ref. [6] argues for the \( d/4 \) decay exponent. In ref. [19] it was incorrectly concluded that dressed-tree calculation results in the \( d/2 \) exponent, which basically came from balancing wrong terms in Laplace transformed version of Eq. (62). In here calculation done in ref. [19] will be repeated to show how to balance terms correctly. Also, calculation will justify approximations employed in ref. [6] more rigorously as the method of calculation employs Laplace Transform and well known Tauberian theorems which relate small \( s \) with large \( t \) behavior. In this way all the approximations are controlled.

To extract asymptotic behavior for \( n(t) \) from Eq. (62) one assumes that at large times density decays as

\[ n(t) \approx A(\mu + t)^{-\alpha} \quad (63) \]

\( A \) and \( \alpha \) denote amplitude and exponent of decay to be found. \( \mu \) is introduced as regulator for small \( t \) so that Laplace transform of \( n(t) \) and \( n^2(t) \) exist;

\[ n(s) = Ae^{\mu s} s^{\alpha-1} \Gamma(1-\alpha, ms) \quad (64) \]
\[ n_2(s) = A^2 e^{\mu s} s^{2\alpha-1} \Gamma(1-2\alpha, ms) \quad (65) \]

and please note that \( n(s)^2 \neq n_2(s) \). To extract asymptotics one inserts (64)-(65) and (61) into (60) and expands in small \( s \) (to extract leading order behavior for large \( t \)) and matches the most dominant terms.

The expansion of \( g(s) \) for small \( s \) is given by

\[ g(s) = (8\pi D)^{-d/2} e^{\eta s} \times \left[ \Gamma(1-d/2) s^{d/2-1} + \frac{2\eta^{1-d/2}}{d-2} + \mathcal{O}(s) \right] \quad (66) \]

for \( d \neq 2, 4, 6, \ldots \). For \( d = 2 \) one has

\[ g(s) = (8\pi D)^{-1} e^{\eta s} [-\gamma_E - \ln(\eta s) + \mathcal{O}(\eta s)] \quad (67) \]

where \( \gamma_E \) is Euler constant. Please note that the behavior of \( g(s) \) for small \( s \) is qualitatively different for \( d < 2 \) and \( d > 2 \) which has to do with recurrence of random walks bellow and above \( d = 2 \). For small \( s \) and \( d < 2 \) \( g(s) \propto s^{d/2-1} \) while for \( d > 2 \) \( g(s) = \text{const} \). At \( d = 2 \) there is logarithmic dependence on \( s \). The term \( e^{\eta s} \) can be neglected if leading order behavior for small \( s \) (large \( t \)) is sought for.

At the moment we focus on the \( d < 2 \) case. Inserting approximate formulas above for \( g(s) \) into (61) gives

\[ \lambda_{\text{eff}}(s) \sim \frac{(8\pi D)^{d/2}}{\Gamma(1-d/2)} s^{d/2+1}, \quad d < 2 \quad (68) \]

Since value for \( \alpha \) is not known one has to separate various cases: expansion for \( n(s) \) reads

\[ n(s) = A \left\{ \begin{array}{ll}
\Gamma(1-\alpha) s^{\alpha-1} + \mathcal{O}(1) & \alpha < 1 \\
\frac{\Gamma(1-\alpha) s^{\alpha-1}}{\Gamma(1-\alpha)} + \mathcal{O}(s^{\alpha-1}) & \alpha > 1
\end{array} \right. \quad (69) \]

and likewise for \( n_2(s) \)

\[ n_2(s) = A^2 \left\{ \begin{array}{ll}
\Gamma(1-2\alpha) s^{2\alpha-1} + \mathcal{O}(1) & 2\alpha < 1 \\
\frac{\Gamma(1-2\alpha) s^{2\alpha-1}}{\Gamma(1-2\alpha)} + \mathcal{O}(s^{2\alpha-1}) & 2\alpha > 1
\end{array} \right. \quad (70) \]

Inserting small \( s \) expansions (68)-(70) into (60) gives

\[ A[s^{\alpha} \Gamma(1-\alpha) + \mathcal{O}(s)] - n_0 = -A^2 \frac{(8\pi D)^{d/2}}{\Gamma(1-d/2)} \left[ s^{2\alpha-d/2} \Gamma(1-2\alpha) + \mathcal{O}(s^{1-d/2}) \right] \quad (71) \]

Also, please note that there are two different forms to use for \( n(s) \) and \( n_2(s) \) in (69) and (70) and the ones used in (71) were for \( \alpha < 1 \) and \( 2\alpha < 1 \) respectively (same choice was made in ref. [19]). Once \( \alpha \) is found, one has to check these conditions on \( \alpha \) for self consistency. There are two ways to match the terms in (71), (a) as in the ref. [19], and (b) in a way related to the work in ref. [6]. We begin with first case.

Balancing \( s^{\alpha} \) term on the left hand side of (71) with \( s^{2\alpha-d/2} \) on the right hand side, gives \( \alpha = d/2 \) and

\[ A_{\alpha} = -\frac{1}{\pi} \sin(\pi d) \Gamma(d) \Gamma(1-d/2)^2 (8\pi D)^{-d/2} \quad (72) \]

Also from \( \alpha < 1 \) and \( 2\alpha < 1 \) one has constraint that \( d < 1 \). However, for \( d < 1 \) the term \( \sin(\pi d) \) is positive which makes amplitude \( A_{\alpha} \) negative. Thus all physical conditions can not be met with this type of matching. In ref. [19] the condition \( d < 1 \) [coming from the fact that first row is used in (70)] was overlooked (if \( d > 2 \) is allowed amplitude \( A_{\alpha} \) is perfectly acceptable).

The \( \alpha = d/2 \) scenario can still turn out to be true. With this choice of \( \alpha \) and \( d < 2 \) condition coming from (68) the second row in (70) have to be used. Again, carrying out similar type of matching procedure would give negative amplitude. Finally, the \( \alpha = d/2 \) avenue has to be given up.
At this stage one is left by the second (b) way of balancing, i.e. matching constant \( n_0 \) term on the left hand side of (71) with \( s^{2α-d/2} \) on the right hand side. (The remaining terms, e.g. such as the \( s^n \) on the left hand side can be balanced by considering sub-leading corrections to \( n(s) \)). This way of balancing immediately gives \( α = d/4 \) and

\[
A_b = \sqrt{n_0(8\pi D)}^{-d/4}
\]

with constraints that \( d < 2 \) (Eq. 68 was used to get Eq. 71).

Matching the constant term \( n_0 \) on the left hand side of (71) is rather counter-intuitive since in the framework of Laplace transform constant can normally be disregarded when large \( t \) behavior is sought for. To see how this comes about it is useful to turn back to Eq. (60).

Equation (60) comes from Eq. (57). For simplicity reasons we focus on the case \( \lambda = \infty \) in (57). It is clear that at the right hand side of equation (57) the \( sn(s) \) term is sub-leading to \( n_0 \). (True enough, \( n_0 \) is constant but it is multiplied by \( g(s) \).) Thus \( n_2(s) \) indeed has to be matched with \( g(s)n_0 \). This procedure results in amplitude \( A_b \) obtained previously. Also, by using form (57), one can show that amplitude \( A_b \) as given in Eq. (73) is valid even for \( d > 2 \). Analysis can be repeated with finite value of \( \lambda \) with the same outcome. Before proceeding, it is important to mentioned that procedure outlined above does not work at \( d \geq 4 \) and it has to be modified.

The main findings of this subsection are twofold. First, it has been shown that dressed tree calculation is equivalent to WBGA-I. Second, it was shown that WBGA-I (and dressed tree calculation) fail to describe A+A reaction predicting \( d/4 \) decay exponent:

\[
n(t) \sim \sqrt{n_0(8\pi Dt)}^{-d/4}
\]

All findings of this subsection are summarized in Fig. 1. The numerical treatment of Eqs. (54) and (55) confirms asymptotic decay given in Eq. (74). Equations (54) and (55) were solved previously numerically in ref. [6]. In here, the features of the decay curves are somewhat different from the ones obtained in ref. [6]. For example, curves shown in this work have concave form (bend upward), while curves in fig. 1 of ref. [6] are convex (bend downward) as if asymptotics have not yet been reached. Also, in here, there is no intersection of curves, which can be found in ref. [6]. These difference could come from the numerical treatment. Apart from using double precision, to obtain curves in Fig. 1 the method of integration was used which integrates exactly \( \int_0^t dt'(t-t')^{-d/2}f(t') \) provided \( f(t) \) is piecewise linear in \( t \). The more detailed description of numerical treatment is shown in the appendix B.

In the next subsection it will be shown that, in the case of A+A reaction, weaknesses of WBGA-I method extend to WBGA-II level.

### B. The WBGA-II approximation

When term \( n\Gamma_k \) is kept in Eq. (48), equivalent of Eq. (55) reads

\[
\varphi(t) = n(t)^2 - \lambda \int_0^t dt'I(t,t')\varphi(t')
\]

while Eq. (54) stays the same. The \( I(t,t') \) is given by

\[
I(t,t') = G(t-t') exp \left[-4\lambda \int_0^t dt''n(t'')\right]
\]

The asymptotics of Eq. (75) can not be extracted by Laplace transform, and it is more convenient to use approach of ref. [6]. For large \( t \), Eq. (75) can be approximated by

\[
\varphi(t) \approx n(t)^2 - I(t,0)\mathcal{I}(t)
\]

where \( \mathcal{I}(t) = \lambda \int_0^t dt'\varphi(t') \). This step is valid provided both conditions are satisfied. First, the term \( I(t,t') \) has to vanish as time difference \( t - t' \) grows. Second, the integral \( \int_0^t dt\varphi(t) \) has to be finite. Using (54) one gets \( \mathcal{I}(t) = n(t) - n(t) \approx n_0 \) and (77) becomes

\[
\frac{∂n}{∂t} \approx -λn^2 + \lambda I(t,0)n_0
\]

Equation above is solved with the assumption that asymptotically \( n(t) \sim A/t \), which is checked self consistently at the end. Using postulated asymptotics for \( t \), one can see from Eq. (76) that \( I(t,0) \sim \text{const} t^{-(d/2 + 4\lambda A)} \). Assuming that

\[
\frac{I(t,0)}{n(t)^2} \to 0, \quad t \to \infty
\]

one can solve (78) in form \( ∂n/∂t = -λn^2 \), and get \( A = 1/λ \). Assumption (79) is correct provided \( 2 < d/2 + 4\lambda A = d/2 + 4 \), which is true for any \( d \). This shows that \( n(t) \approx 1/(λt) \) is asymptotic form for the solution of Eqs. (54) and (75). This means that the last term \( (n\Gamma_k) \) in (48) only influences intermediate behavior when \( t \) is not too large. For large \( t \), WBGA-II gives exactly the same asymptotics as the pure mean field treatment.

Thus main finding so far is that both WBGA-I and WBGA-II fail to describe A+A reaction. This is somewhat surprising as even simplest pair-approach, e.g. Smoluchowski method, describes exponent of A+A correctly. Clearly A+A reaction can not be viewed as a weakly interacting Bose-gas. The question is what is the minimum modification of WBGA which will provide correct result for the A+A model? This question will be answered in the next subsection.
C. The hybrid of WBGA and Kirkwood superposition approximation

To see how to improve WBGA one has to clarify what went wrong in the first place. We start from problematic equation (40) which becomes (48) when terms with $\sigma^A_{kB}$ are set to zero. To trace why WBGA fails it is useful to rewrite Eq. (40) as it looks one step before WBGA is made, and we keep only terms describing A+A reaction:

$$\frac{\partial}{\partial t} \Gamma_k = -2Dk^2\Gamma_k - \left[ \sigma_k n^2 + \frac{1}{V} \sum_{q \neq k} \sigma_q \Gamma_{k-q} \right] - \hat{\Gamma}^{(3)}$$ (80)

where

$$\hat{\Gamma}^{(3)} = \frac{1}{V} \sum_q \sigma_q \left( \langle a_{k} a_{k-q} a_q \rangle + \langle a_k a_{k-q} a_q \rangle \right)$$ (81)

is focus of present subsection. In technical terms, the usage of WBGA can be translated into approximating three point density $\langle a_x a_y a_z \rangle$ in a particular way. In the case of WBGA-I one simply takes

$$\langle a_k a_k a_k \rangle = \langle a_x a_y a_z \rangle = 0$$ (82)

while in WBGA-II one assumes

$$\langle a_k a_k a_k \rangle \approx \delta_{k_1,0} \delta_{k_2,0} \delta_{k_3,0} a_0^3 + \delta_{k_1,0} \delta_{k_2,0} \delta_{k_3,0} a_0 \langle a_k a_k a_k \rangle + \delta_{k_1,0} \delta_{k_2,0} \delta_{k_3,0} a_0 \langle a_k a_k a_k \rangle + \delta_{k_1,0} \delta_{k_2,0} \delta_{k_3,0} a_0 \langle a_k a_k a_k \rangle$$ (83)

where $\delta_{k,0} \equiv 1 - \delta_{k,0}$. Inserting (83) into (80) gives the terms describing A+A process in (40). It is useful to transform approximation above into the x-space to understand nature of approximation better. Inverse Fourier transform of (83) gives [25]

$$\langle a_x a_y a_z \rangle \approx n^3 + n \langle a_x a_y \rangle - n^2 + n \langle a_x a_z \rangle - n^2 + n \langle a_y a_z \rangle - n^2$$ (84)

The WBGA approximations given in Eqs. (82) and (84) can be contrasted to the Kirkwood superposition approximation,

$$\langle a_x a_y a_z \rangle \approx \frac{1}{n^3} \langle a_x a_y \rangle \langle a_x a_z \rangle \langle a_y a_z \rangle$$ (85)

which is known to describe A+A problem correctly (at least the decay exponent).

It is interesting to note that instead of (85) one could carry out Kirkwood superposition approximation in a different way, e.g. as $\langle n_x n_y n_z \rangle \approx \langle n_x n_y \rangle \langle n_x n_z \rangle \langle n_y n_z \rangle / n^3$. (There is no such ambiguity when only single occupancy of site is allowed.) When multiple site occupancy is allowed, as considered here, we argue that Eq. (85) is more accurate way to implement Kirkwood superposition approximation.

By looking at equation (84) it is possible to understand WBGA better. Eq. (84) suggests that WBGA is somewhat equivalent to the additive expansion of correlation functions. It has been argued that such additive approximation is inferior to the Kirkwood superposition approximation [4,5]. This in turn explains why WBGA fails to describe the A+A reaction.

Clearly, to correctly describe A+A reaction one has to use Kirkwood superposition approximation, which we modify further in the spirit of WBGA, assuming that higher order products of annihilation operators $a_k, b_k$ with $k \neq 0$ are small, and accounting for thermodynamic limit (extracting $a_0$ or $b_0$ out of field theoretic averages). This is done in two stages. First, Kirkwood superposition approximation in Eq. (85) is rephrased in the k-space which gives [26]

$$\langle a_k a_k a_k \rangle \approx \delta(1 + k + k) \sum_l \Gamma_{k-l+1}$$ (86)

To get the improved form for three body terms one inserts (86) into (81) which gives

$$\hat{\Gamma}^{(3)} \approx \frac{2}{n^3 V^2} \sum_{l} \sigma_q \Gamma_{k+l} \Gamma_{k+q-l}$$ (87)

The expression above was obtained by using symmetry properties of $\Gamma_k = \Gamma_{-k}$ and $\sigma_q = \sigma_{-q}$. Also upon inserting (86) into (81) the two terms on the right hand side of (81) contribute equally resulting in factor two in (87). Equation above is too complicated to be used in practise and we approximate it further.

In the spirit of WBGA the terms in (86) which contain large number of correlation functions with k-vector different from zero are neglected. This is done in two stages, first sum over $q$ is split into $q = k$ and $q \neq k$ parts, and then for each of sums various contributions from sum over $l$ are distilled to extract non-fluctuating $k = 0$ operators. This gives

$$\hat{\Gamma}^{(3)} \approx \frac{2}{n^3 V^2} \left[ \Gamma_k (\Gamma_0 \Gamma_k + \Gamma_0 \Gamma_k) + \sum_{l \neq k} \sigma_q \Gamma_0 (\Gamma_k \Gamma_{l-k} + \Gamma_k \Gamma_{q-l-k}) \right]$$ (88)

where terms of the type $\Gamma_k \Gamma_q$ with $k, q, l \neq 0$ have been neglected. Eq. (88) is still complicated to be used, at least to obtain analytic result. First term on the right hand side of (88) can be neglected since it leads to mean field behavior (as shown in section IV B). Second term can be absorbed into the one of the three terms under the
sum sign, e.g. under the first term. Second and third terms under the sum sign couple correlation functions in a non-trivial way and are neglected in the following for simplicity reasons. With \( \Gamma_0 \approx n^2V \), and applying recipe just described gives

\[
\Gamma^{(3)} \approx \frac{2}{nV} \Gamma_k \sum_q \sigma_k \Gamma_q \tag{89}
\]

which is midway between WBGA-II (Eq. 83) and Kirkwood superposition approximation (Eq. 86). It is interesting to note that equation above is very close to the shortened Kirkwood superposition approximation discussed in refs. [4,5]. Using approximation above to decouple three body density, and particular form for \( \sigma_{xy} \) used throughout this section, gives following equations of motion,

\[
\frac{\partial}{\partial t} \Gamma_k = -2Dk^2\Gamma_k - \lambda(n^2 + \Phi) - 2\lambda \Gamma_k \frac{\Phi + n^2}{n} \tag{90}
\]

which should be contrasted with Eq. (48). The most convenient way to solve (47) and (90) is to introduce \( \chi_k \) as \( \Gamma_k = n^2\chi_k \) and \( \Phi = n^2\chi \) where

\[
\chi \equiv 1 + \frac{1}{V} \sum_{k \neq 0} \chi_k \tag{91}
\]

\( \chi_k \) with \( k = 0 \) is set equal to \( V \) and does not change in time (thermodynamic limit). Applying change of variables just described modifies Eq. (47) into

\[
\frac{\partial}{\partial t} n(t) = -\kappa(t)n(t)^2 \tag{92}
\]

where effective reaction rate

\[
\kappa(t) = \lambda \chi(t) \tag{93}
\]

was introduced. Same change of variables transforms Eq. (90) into

\[
\frac{\partial}{\partial t} \chi_k = -2Dk^2\chi_k - \lambda \chi \tag{94}
\]

Equation (94) can be solved for all \( \chi_k \) and \( k \neq 0 \) (pretending that \( \chi(t) \) is known), and after summing over \( k \neq 0 \) one gets following integral equation

\[
\chi(t) = 1 - \lambda \int_0^t dt' G(t - t') \chi(t') \tag{95}
\]

Solution of the equation above can be found by Laplace transform which gives

\[
\kappa(s) = \frac{\lambda}{s[1 + \lambda g(s)]} \tag{96}
\]

Also, one can integrate Eq. (92) which gives

\[
n(t) = \frac{n_0}{1 + n_0 \kappa(t)} \quad \tilde{\kappa}(t) = \int_0^t dt' \kappa(t') \tag{97}
\]

It is not possible to obtain closed expression for \( \kappa(t) \) and \( n(t) \). However, asymptotic form of \( n(t) \) can be extracted.

Inserting small \( s \) expansion of \( g(s) \) (see Eqs. 66 and 67) into (96) gives

\[
\kappa(s) \sim \begin{cases} \frac{(8\pi D)s^{d/2}}{\Gamma(1-d/2)} & d < 2 \\ -\frac{8\pi D}{s^\lambda[\lambda + \ln(qs)]} & d = 2 \\ \lambda \frac{\kappa}{1 + \lambda g(0)} s^{-1} & d > 2 \end{cases} \tag{98}
\]

for \( s \to 0 \). Taking inverse Laplace transform of equation above gives leading order behavior for effective reaction rate constant,

\[
\kappa(t) \sim \begin{cases} \frac{\Gamma(1-d/2)}{\Gamma(1-d/2)[1-(d/2)]} t^{d/2-1} & d < 2 \\ \frac{8\pi D}{\ln^{d/2}q} & d = 2 \\ \left[\frac{\lambda}{\kappa + g(0)}\right] t^{-1} & d > 2 \end{cases} \tag{99}
\]

when \( t \to \infty \). To find inverse Laplace transform of \( \kappa(s) \) for \( d = 2 \) (second line Eq. 98) is somewhat involved, please see appendix C for details. Finally, inserting (99) into (97) gives asymptotics

\[
n(t) \sim \begin{cases} \Gamma(1-d/2)[1 + d/2](8\pi Dt)^{-d/2} & d < 2 \\ \frac{\ln^{(d/2)}q}{8\pi Dt} & d = 2 \\ \left[\frac{\lambda}{\kappa + g(0)}\right] t^{-1} & d > 2 \end{cases} \tag{100}
\]

where \( g(0) \) entering in the third row can easily be found from (66).

V. WBGA APPLIED TO THE A+B REACTION

Equations of motion for density and correlation functions describing A+B model result from (35)-(36) and (40)-(42) by using (46) with \( \lambda = 0 \). For simplicity reasons, we focus on \( n_A = n_B = n \) case and omit labels A and B. Also, as in the previous section \( n_0 = n_{0,A} = n_{0,B} \). Applying procedure outlined above leads to the equations for particle densities

\[
\frac{\partial n}{\partial t} = -\delta(n^2 + \Phi_c) \tag{101}
\]

where \( \Phi_c \) is given by the AB correlation function,
Equations for correlators $\Gamma_k \equiv \Gamma_k^A = \Gamma_k^{BB}$ and $\Gamma_k^c \equiv \Gamma_k^{AB}$ are given by

$$\left( \frac{\partial}{\partial t} + 2Dk^2 \right) \Gamma_k = -\delta(n^2 + \Phi_c) - 2\delta n(\Gamma_k + \Gamma_k^c)$$  \hspace{1cm} (103)

$$\left( \frac{\partial}{\partial t} + 2Dk^2 \right) \Gamma_k = -2\delta n(\Gamma_k + \Gamma_k^c)$$  \hspace{1cm} (104)

The most convenient way to solve equations above is to diagonalise them by subtraction and addition. The final result is that correlations of AB pairs are governed by

$$\Phi_c(t) = \frac{1}{V} \sum_{k \neq 0} \Gamma_k^{AB}(t)$$  \hspace{1cm} (102)

Equations for correlators $\Gamma_k \equiv \Gamma_k^A = \Gamma_k^{BB}$ and $\Gamma_k^c \equiv \Gamma_k^{AB}$ are given by

$$\left( \frac{\partial}{\partial t} + 2Dk^2 \right) \Gamma_k = -\delta(n^2 + \Phi_c) - 2\delta n(\Gamma_k + \Gamma_k^c)$$  \hspace{1cm} (103)

$$\left( \frac{\partial}{\partial t} + 2Dk^2 \right) \Gamma_k = -2\delta n(\Gamma_k + \Gamma_k^c)$$  \hspace{1cm} (104)

The most convenient way to solve equations above is to diagonalise them by subtraction and addition. The final result is that correlations of AB pairs are governed by

$$\Phi_c(t) = -\delta \int_0^t dt' [G(t, t') + I(t, t')][n(t')^2 + \Phi_c(t')]$$  \hspace{1cm} (105)

and for AA (or BB) pairs as

$$\Phi(t) = \delta \int_0^t dt' [G(t, t') - I(t, t')] [n(t')^2 + \Phi_c(t')]$$  \hspace{1cm} (106)

The $I(t, t')$ appearing in equations (105) and (106) has the same form as in (76) with trivial change of $\lambda$ into $\delta$. Same type of analysis as in the subsection IVB leads to conclusion that approximation $G(t, t') + I(t, t') \approx G(t, t')$ can be used, which in turn leads to $d/4$ density decay exponent. Interestingly enough, both WBGA-I and WBGA-II approaches lead to correct $d/4$ exponent when used to solve A+B model.

In some sense the WBGA approach seems to be suited rather well for A+B reaction. Quite the contrary can be said for A+A reaction as shown previously. To understand workings of WBGA on the more general model the ABBA model will be studied in the next section.

**VI. WBGA APPLIED TO THE ABBA MODEL**

The ABBA model was suggested in refs. [14,15] and it has a number of interesting properties. The model is obtained as the special case of the general two species model discussed in section II where A+A and B+B reactions occur with same reaction rate $\lambda$, while A+B with reactions rate $\delta$, and $\delta > \lambda$ is taken. The fact that A and B species have equal diffusion constants is very important since it leads to survival of minority species. Minority species is the one with smaller concentration at $t = 0$, and we chose B to be minority, i.e. $n_{0,B} > n_{0,A}$. By survival it is meant that particle density ratio saturates to constant $u(t) \equiv n_A(t)/n_B(t) \rightarrow \text{const}$ as $t \rightarrow \infty$. (The mean field analysis predicts vanishing of minority species $u(t) \rightarrow \infty$ as $t \rightarrow \infty$. Also, similar model has been studied in ref. [27] where it was shown that if $D_A \neq D_B$ only one type of species survives.)

The goal of the present section is to understand strengths and weaknesses of WBGA approach by testing it on the ABBA model which combines A+A and A+B reactions. These reactions have been studied in previous sections but now they are allowed to occur simultaneously. It is interesting to see how WBGA approach performs in such situation. Clearly, there are plenty of possibilities how to combine A+A and A+B reactions, but the way they are combined in the ABBA model gives rise to many interesting effects. (For example, there is survival of minority species, recovery of initial density ratio, dependence of amplitudes on initial densities and reaction rates [28], please see refs. [14,15] for details).

We start from equations of motion given in section III which describe very general two species reaction-diffusion model. Equations for correlators (40)-(42) simplify to

$$\frac{\partial}{\partial t} n_A = -\left( \lambda n_A^2 + \delta n_A n_B + \lambda \Phi_{AA} + \delta \Phi_{AB} \right)$$  \hspace{1cm} (107)

$$\frac{\partial}{\partial t} n_B = -\left( \lambda n_B^2 + \delta n_A n_B + \lambda \Phi_{BB} + \delta \Phi_{AB} \right)$$  \hspace{1cm} (108)

where

$$\Phi_{\rho\sigma} = \frac{1}{V} \sum_{k \neq 0} \Gamma_k^{\rho\sigma}$$, \hspace{1cm} $\rho, \sigma = A, B$  \hspace{1cm} (109)

Also, Eqs. for correlators (40)-(42) simplify to

$$\frac{\partial}{\partial t} \Gamma_k^{AA} = -2Dk^2 \Gamma_k^{AA} - \lambda \left( n_A^2 + \Phi_{AA} \right) - 2(2\lambda n_A + \delta n_B) \Gamma_k^{AA} - 2\delta n_A \Gamma_k^{AB}$$  \hspace{1cm} (110)

$$\frac{\partial}{\partial t} \Gamma_k^{BB} = -2Dk^2 \Gamma_k^{BB} - \lambda \left( n_B^2 + \Phi_{BB} \right) - 2(2\lambda n_A + \delta n_B) \Gamma_k^{BB} - 2\delta n_B \Gamma_k^{AB}$$  \hspace{1cm} (111)

$$\frac{\partial}{\partial t} \Gamma_k^{AB} = -2Dk^2 \Gamma_k^{AB} - \delta (n_A n_B + \Phi_{AB}) - (2\lambda + \delta)(n_A + n_B) \Gamma_k^{AB} - 2\delta n_A \Gamma_k^{AB}$$  \hspace{1cm} (112)

The equations above will be solved in the next two subsections within WBGA-I and WBGA-II approaches.

**A. The WBGA-I approximation**

In the framework of WBGA-I all seemingly $O(n^3)$ terms of the type $n_\rho \Gamma_k^{\rho\sigma}$ with $\rho = A, B$ and $\sigma = AA, AB, BB$ are thrown away in (110)-(112). Following similar steps as in subsection IV A gives
\[
\frac{\partial}{\partial t} n_A = -(\lambda \varphi_{AA} + \delta \varphi_{AB}) \tag{113}
\]
\[
\frac{\partial}{\partial t} n_B = -(\lambda \varphi_{BB} + \delta \varphi_{AB}) \tag{114}
\]

and
\[
\varphi_{AA} = n_A^2 - \lambda \int_0^t \! dt' G(t-t') \varphi_{AA}(t') \tag{115}
\]
\[
\varphi_{BB} = n_B^2 - \lambda \int_0^t \! dt' G(t-t') \varphi_{BB}(t') \tag{116}
\]
\[
\varphi_{AB} = n_A n_B - \delta \int_0^t \! dt' G(t-t') \varphi_{AB}(t') \tag{117}
\]

where \( \varphi_{\rho \nu} \equiv n_\rho n_\nu + \Phi_{\rho \nu} \) for \( \rho, \nu \in \{A, B\} \). To solve Eqs. (113)-(116) it is possible to employ same technique as in section IV B. Equations above can be approximated by
\[
0 \approx n_A^2 - G(t,0) I_{AA}(t) \tag{118}
\]
\[
0 \approx n_B^2 - G(t,0) I_{BB}(t) \tag{119}
\]
\[
0 \approx n_A n_B - G(t,0) I_{AB}(t) \tag{120}
\]

where
\[
I_{\rho \nu}(t) \equiv (\lambda \delta_{\rho, \nu} + \delta \delta_{\rho, \nu}) \int_0^t \! dt' \varphi_{\rho \nu}(t') , \quad \rho = A, B \tag{121}
\]

By integrating Eqs. (113) and (114) a useful relationship can be derived for \( I_{\rho \nu} \), \( \rho, \nu = A, B \):
\[
I_{AA}(t) + I_{AB}(t) = n_{0,A} - n_A(t) \approx n_{0,A} \tag{122}
\]
\[
I_{BB}(t) + I_{AB}(t) = n_{0,B} - n_B(t) \approx n_{0,B} \tag{123}
\]

Using (118)-(120) gives \( (n_A + n_B)^2 \approx G(t)(I_{AA} + I_{BB} + 2I_{AB}) \), and adding (122) and (123) finally gives
\[
(n_A + n_B)^2 \approx G(t)(n_{0,A} + n_{0,B}) \tag{124}
\]

Also from (118) and (119) \( n_A^2 - n_B^2 \approx G(t)(I_{AA} - I_{BB}) \) and subtraction of (122) and (123) gives
\[
n_A^2 - n_B^2 \approx G(t)(n_{0,A} - n_{0,B}) \tag{125}
\]

After solving (124) and (125) for \( n_A \) and \( n_B \) one gets
\[
n_\rho \sim \frac{n_\rho(0)}{\sqrt{n_{0,A} + n_{0,B}}} (8\pi Dt)^{-d/4} , \quad \rho = A, B \tag{126}
\]

According to WBGA-I both particles decay with \( d/4 \) exponent and amplitudes given above. The WBGA-I predicts same decay exponent as for the pure A+A model. As in the case of A+A reaction, the value for \( d/4 \) exponent obtained here is not correct. The computer simulation and \( \epsilon \)-expansion analysis of this reaction suggest \( d/2 \) exponent [14,15]. To see what happens when \( O(n^3) \) terms are kept in (110)-(112) we proceed with WBGA-II calculation.

B. The WBGA-II approximation

In the WBGA-II approximation, when all terms are kept in Eqs. (110)-(112), it is useful to rewrite these equations in the vector form
\[
\begin{pmatrix}
\frac{\partial}{\partial t} + 2Dk^2 \Gamma_k^4
\end{pmatrix}
\begin{pmatrix}
\Gamma_k^4
\end{pmatrix}
= -P(t)
\begin{pmatrix}
\Gamma_k^{AB}
\end{pmatrix}
- \begin{pmatrix}
\lambda \varphi_{AA}
\lambda \varphi_{BB}
\delta \varphi_{AB}
\end{pmatrix}
\tag{127}
\]

where the matrix \( P \) is given by
\[
P = n_A
\begin{pmatrix}
4\lambda + 2\delta u & 0 & 2\delta \\
0 & 4\lambda u + \delta & 2\delta u \\
\delta & 2(\lambda + \delta) & (1 + u)
\end{pmatrix}
\tag{128}
\]
with \( u = n_B/n_A \).

Vector equation (127) is very hard to solve analytically. However, there are some guidelines how to extract late time asymptotics. At the WBGA-I level it appears that ABBA model and the A+A model are very similar. In the following it will be assumed that such similarity can be extrapolated to the presently studied WBGA-II level. This implies that mean field behavior should be expected from Eq. (127).

To get the feeling for what follows it is useful to analyze Eqs. (107) and (108) at the mean field level by neglecting fluctuations and setting \( \Phi_{\rho \nu} \) to zero with \( \rho, \nu = A, B \). Carrying out such procedure gives
\[
\frac{\partial}{\partial t} n_A = -(\lambda n_A^2 + \delta n_A n_B) \tag{129}
\]
\[
\frac{\partial}{\partial t} n_B = -(\lambda n_B^2 + \delta n_A n_B) \tag{130}
\]

Equations above can be solved approximatively for large \( t \) (please see refs. [15] for details) and one obtains
\[
n_A \sim \frac{1}{\lambda t} \tag{131}
\]
\[
n_B \sim \frac{n_{0,B}}{|n_{0,A} \lambda t|} \tag{132}
\]
provided \( \gamma \equiv \delta/\lambda > 1 \) and \( n_{0,A} > n_{0,B} \). For \( \delta = \lambda \) (\( \gamma = 1 \)) or \( n_{0,A} = n_{0,B} \) solution is trivial, and it can be easily shown that in such case the ABBA model belongs to the A+A universality class. These simple cases are not
considered here. Initial imbalance in particle concentration leads to faster diminishing of minority species, i.e. \( u(t) = n_B(t)/n_A(t) \to 0 \) as \( t \to \infty \) given \( 0 < u(0) < 1 \).

In the following we assume the mean field ansatz (131)-(132) and try to solve (127) with it. The validity of such mean field ansatz will be checked self consistently at the end. For large times, and with mean field behavior \((u \to 0)\), the matrix \( P \) can be approximated by

\[
P \approx \lambda n_A \Pi \tag{133}
\]

with

\[
\Pi = \begin{pmatrix}
4 & 0 & 2\gamma \\
0 & 2\gamma & 0 \\
0 & \gamma & 2 + \gamma
\end{pmatrix} \tag{134}
\]

The fact that \( P \) (in the approximate form) is constant matrix multiplied by time dependent function implies that \([P(t), P(t')] = 0\) (dot over symbol \( P \) denotes time derivative). This being the case, Eq. (127) can be treated as scalar equation and calculation similar to the one in the subsection IV B gives

\[
\begin{pmatrix}
\varphi_{AA}(t) \\
\varphi_{BB}(t) \\
\varphi_{AB}(t)
\end{pmatrix} = \begin{pmatrix}
\frac{n_A(t)^2}{n_B(t)^2} \\
n_A(t)n_B(t) \\
\frac{\lambda \varphi_{AA}(t')}{\delta \varphi_{AB}(t')}
\end{pmatrix} - \int_0^t dt' \begin{pmatrix}
\varphi_{AA}(t') \\
\varphi_{BB}(t') \\
\varphi_{AB}(t')
\end{pmatrix} \tag{135}
\]

where matrix \( J(t, t') \) is given by

\[
J(t, t') = G(t, t') \exp [-\xi(t, t')\Pi] \tag{136}
\]

and

\[
\xi(t, t') = \lambda \int_{t'}^t dt'' n_A(t'') \tag{137}
\]

Please compare Eqs. (75)-(76) and (135)-(136). They are very similar, the only difference being in the matrix character of (135-136). Following same steps as in section IV B the Eq. (135) can be approximated as

\[
\begin{pmatrix}
\varphi_{AA} \\
\varphi_{BB} \\
\varphi_{AB}
\end{pmatrix} \approx \begin{pmatrix}
n_A^2 \\
n_B^2 \\
n_A n_B
\end{pmatrix} - \begin{pmatrix}
I_{AA} \\
I_{BB} \\
I_{AB}
\end{pmatrix} J(t, 0) \tag{138}
\]

Now we proceed to show that, as in the case of (77), the second term on the right hand side of equation (138) can be neglected.

Matrix \( \Pi \) can be diagonalized as \( \Pi U = U \Omega \). The \( \Omega \) is diagonal matrix containing eigenvalues \( \omega_1 = 4, \omega_2 = 2\gamma, \omega_3 = 2 + \gamma \) (139)

and matrix \( U \) contains eigenvectors

\[
U = \begin{pmatrix}
1 & \gamma & 2\gamma \\
0 & \gamma & 2\gamma \\
0 & 1 & 1
\end{pmatrix} \tag{140}
\]

Inserting (131) into (137), and assuming large \( t \), leads to

\[
\xi(t, 0) \sim const + \ln t \tag{141}
\]

and using (141) in (136) gives

\[
J(t, 0) \sim const t^{-d/2} U \begin{pmatrix}
t^{-4} & 0 & 0 \\
0 & t^{-2\gamma} & 0 \\
0 & 0 & t^{-(2+\gamma)}
\end{pmatrix} U^{-1} \tag{142}
\]

Finally, the second term on the right hand side of (138) can be calculated explicitly. Inserting (142) into (138), and assuming that \( I_{\rho\nu} \rho, \nu = A, B \) are constants (can be checked for self consistency at the end), results in

\[
\begin{align*}
\varphi_{AA} & \approx n_A^2 + t^{-d/2}(c_1 t^{-\omega_1} + c_2 t^{-\omega_2} + c_3 t^{-\omega_3}) \\
\varphi_{BB} & \approx n_B^2 + t^{-d/2} c_4 t^{-\omega_2} \\
\varphi_{AB} & \approx n_A n_B + t^{-d/2} (c_5 t^{-\omega_2} + c_6 t^{-\omega_2})
\end{align*} \tag{143-145}
\]

The explicit form of constants \( c_1, c_2, c_3, c_4, c_5 \) and \( c_6 \) is not interesting since aim is to show that terms containing these constants are sub-leading to the mean field terms. By studying equation above row by row, it is possible to show that for \( \gamma \geq 1 \) terms involving constants are sub-leading to the mean field terms.

To see that terms originating from \( J(t, 0) \) are sub-leading one really has to calculate \( U \) explicitly. For example, not knowing that contribution from \( \omega_1 \) is absent in (144), there would be a need to compare \( t^{-2\gamma} \) (asymptotics of the mean field \( n_B^2 \) term in 144) with \( t^{-(d/2+4)} \) (coming from \( J(t, 0) \) and \( \omega_1 \) eigenvalue). One would conclude that \( \gamma = \delta/\lambda \) can not be too large if mean field asymptotics is to hold. In reality, there is no such bound on ratio \( \delta/\lambda \) since eigenvalue \( \omega_1 \) does not appear in Eq. (144), but this can only be seen after explicit calculation.

Main findings so far is that WBGA describes ABBA and A+A model in the same way. For both models the WBGA-I (WBGA-II) predict \( d/4 \) (mean field) density decay exponents. In the next section attempt will be made to improve WBGA method in order to obtain correct value of density decay exponent for ABBA model.
C. The hybrid of WBGA/Kirkwood applied to A+A and B+B sectors

How deep the weakness of WBGA goes? What needs to be changed in equations of motion (110)-(112) in order to get correct decay exponent? To answer these questions we begin by modifying the A+A and B+B reaction sectors in (110)-(112) by using the recipe from section IV C. It was already remarked in the section II that contributions to H describing different reaction sectors enter additively, and this feature is reflected in equations of motion (110)-(112). Because of this it is possible to focus on terms describing influence of A+A and B+B reactions, i.e. terms proportional to \( \lambda \), which govern decay exponents of the ABBA model. At the moment terms proportional to \( \delta \) in (110)-(112) that describe A+B reaction will not be changed.

If one is to follow procedure described in section IV C, the \( O(n^3) \) term in Eq. (110) has to be modified as

\[
4\lambda n_A \Gamma_k^{AA} \rightarrow 2\lambda \Gamma_k^{AA} n_A^2 + \Phi_{AA} \quad (146)
\]

and likewise for Eq. (111)

\[
4\lambda n_B \Gamma_k^{BB} \rightarrow 2\lambda \Gamma_k^{BB} n_B^2 + \Phi_{BB} \quad (147)
\]

This gives a new set of, hopefully better, equations:

\[
\frac{\partial}{\partial t} \Gamma_k^{AA} = -2Dk^2\Gamma_k^{AA} - \lambda \left( n_A^2 + \Phi_{AA} \right) - 2\lambda \Gamma_k^{AA} n_A^2 + \Phi_{AA} - 2\delta(n_B \Gamma_k^{AA} + n_A \Gamma_k^{AB}) \quad (148)
\]

\[
\frac{\partial}{\partial t} \Gamma_k^{BB} = -2Dk^2\Gamma_k^{BB} - \lambda \left( n_B^2 + \Phi_{BB} \right) - 2\lambda \Gamma_k^{BB} n_B^2 + \Phi_{BB} - 2\delta(n_A \Gamma_k^{BB} + n_B \Gamma_k^{AB}) \quad (149)
\]

Equation (112) stays the same, although the Eq. (112) contains term proportional to \( \lambda \) which should be modified if one follows the principle outlined above. However, at the moment, Eq. (112) will not be changed.

It is useful to employ similar notation to the one used in section IV B:

\[
\Gamma_k^{\rho\nu} = n_\rho n_\nu \lambda_k^{\rho\nu} \quad (150)
\]

and

\[
\chi_{\rho\nu} = 1 + \frac{1}{V} \sum_{k \neq 0} \chi_k^{\rho\nu} \quad (151)
\]

with \( \rho, \nu = A, B \). Using (150) and (151) in Eqs. (113) and (114) results in

\[
\frac{\partial}{\partial t} n_A = -(\lambda \chi_k^{AA} + \delta n_A n_B \chi_{AB}) \quad (152)
\]

\[
\frac{\partial}{\partial t} n_B = -(\lambda \chi_k^{BB} + \delta n_A n_B \chi_{AB}) \quad (153)
\]

Implementing same notation in Eqs. (148), (149) and (112) gives

\[
\frac{\partial}{\partial t} \chi_k^{AA} = -2Dk^2\chi_k^{AA} - \lambda \chi_k^{AA} - 2\delta n_B (1 - \chi_{AB}) \chi_k^{AB} - 2\delta n_A \chi_k^{AB} \quad (154)
\]

\[
\frac{\partial}{\partial t} \chi_k^{BB} = -2Dk^2\chi_k^{BB} - \lambda \chi_k^{BB} - 2\delta n_A (1 - \chi_{AB}) \chi_k^{AB} - 2\delta n_B \chi_k^{AB} \quad (155)
\]

\[
\frac{\partial}{\partial t} \chi_k^{AB} = -2Dk^2\chi_k^{AB} - \delta \chi_k^{AB} - \delta (n_A \chi_k^{AB} + n_B \chi_k^{AB}) \quad (156)
\]

The numerical solution of the set of equations above is shown in Fig. 2 (dotted line). The full line is a result of Monte Carlo simulation where particle densities are obtained as ensemble averages over 500 runs (simulation is repeated 500 times with a shift in the random number generator). The Eqs. (154)-(156) do not describe ABBA model properly, not even qualitatively, since minority species die out faster (the particle density ratio grows to infinity) while the simulation shows that density ratio should saturate to a constant value (full line). Thus the attempt of modifying terms describing A+A and B+B reaction sector in AA and BB correlation functions by using shortened Kirkwood superposition approximation does not cure weaknesses of WBGA approach. The inspection of individual density decays reveals that the equations above correctly describe decay of majority species, i.e. \( n_A \sim (\text{const})^{-d/2} \), but fail do describe decay of minority species \( n_B \).

In the following more terms will be modified by using Kirkwood superposition approximation. The dash-dot line in Fig. 2 shows a solution of equations (not shown here) obtained from modifying A+A and B+B reaction sectors using shortened Kirkwood superposition approximation in the Eq. (112) describing time evolution of AB correlation function. Equations obtained in this way are identical to the (154)-(156) with only difference that Eq. (156) changes in a way that terms proportional to \( \lambda \) drop out. In Fig. 2 it can be seen that even if all \( \lambda \) proportional terms are modified the density ratio curve climbs to infinity, which indicates that minority species dies out, which is not correct behavior. However, the overall trend
gets better as the dash-dot curve lies bellow dotted one and is pushed towards simulation curve.

To continue this line of incremental changes the equations of motion where studied where even the A+\textit{A} reaction sector was modified using shortened Kirkwood superposition approximation (all terms proportional to \(\delta\) were modified). Equations obtained in this way are same as in (154)-(156) the only difference being in the fact that all seemingly \(O(n)\) terms drop out. Thus in the (154)-(156) only diffusion term and terms \(\lambda_{\text{A}\text{A}}, \lambda_{\text{B}\text{B}}\) and \(\delta_{\text{A}\text{B}}\) are kept in (154), (155) and (156) respectively. These equations are not shown explicitly to save the space but it should be clear how they look like. The numerical solution for this set of equations is shown in Fig. 2 as dashed line. It is possible to analytically extract density decay asymptotics for this truncated set of equations which gives \(n_A(t) \sim (\text{const})t^{-d/2}\) and \(n_B(t) \sim (\text{const}')t^{-d/4}\).

The set of equations where Kirkwood superposition approximation has been applied fully agrees with the numerical simulation much better than the rest which are mixture of WBGA and Kirkwood superposition approximation. This is strong indication that, at least for the ABBA model, the Kirkwood superposition approximation is superior to the WBGA method. For example, in Fig. 2, the trend in all curves improve as the content of superposition approximation is increased in equations of motion (dotted line is worse as it climbs fastest, dash-dot line is a bit better, while only dashed line where superposition approximation is implemented fully saturates to constant). As the goal of the present study is to understand WBGA method better, the more detailed analysis of ABBA reaction based on Kirkwood superposition approximation will be presented in forthcoming publication.

VII. CONCLUSIONS

The goal of this study was to test workings of WBGA and to relate some seemingly independent calculation schemes available in the literature. In particular, this work has addressed few important issues.

(1) It was shown that WBGA-I is equivalent to the dressed tree calculation introduced in ref. [19], and this equivalence holds for any model where particles annihilate in pairs. Furthermore, it was shown that for the A+\textit{A} reaction the dressed tree calculation results in \(d/4\) density decay exponent. Thus the contradictory claims of refs. [19] and [6] have been sorted out.

(2) The WBGA method describes A+\textit{B} reaction well, but does not work for A+\textit{A} and ABBA models, and it is reasonable to expect that there are more models that can not be described by WBGA. In the case of ABBA model WBGA predicts faster vanishing of minority species which is suggestive of the A+\textit{B} like behavior rather than the behavior of the ABBA model as found in refs. [14,15]. This bias towards A+\textit{B} type behavior is very hard to get rid off as successively correcting more and more terms in equations of motion for ABBA model by using Kirkwood superposition approximation results in faster vanishing of minority species. The vanishing of minority species persists until all terms are modified by Kirkwood superposition approximation. The WBGA emphasize A+\textit{B} reaction sector too strongly in the ABBA model.

(3) Findings of this work suggest that formalism employed by Mattis-Glasser in [6] where small \(n_0\) expansion is introduced (and applied to study A+B model) is somewhat questionable. This procedure works on A+B model, but might not work for other models. It can be shown (by rescaling \(a^\dagger n_0 \rightarrow a^\dagger\) and \(a/n_0 \rightarrow a\)) that for the type of models studied in here, the small \(n_0\) approximation of ref. [6] amounts to taking away three body terms in Hamiltonian given in Eq. (21) or (28) (e.g. operators of the type \(a^\dagger a a\) and likewise any mixture of \(a\) or \(b\) operators). The neglect of these terms amounts exactly to WBGA-I approach, i.e. neglect of seemingly \(O(n^3)\) terms in equations of motion for correlation functions; for example, equations (54)-(55) of section IV A (A+\textit{A}), or equations (113)-(117) from section VI A (ABBA). In here it has been shown that WBGA-I set of equations result in incorrect \(d/4\) density decay exponent when used for A+\textit{A} and ABBA models. For these reasons, small \(n_0\) expansion, which effectively means taking away three body term in Hamiltonian, can not be trusted if used beyond A+B model.

(4) The Kirkwood superposition approximation was formulated for the case of lattice dynamics with multiple occupancy of lattice sites allowed. There is strong indication from the present analysis that Kirkwood superposition approximation is superior to the WBGA method, at least when applied to the A+\textit{A} and ABBA models. However, one has to be careful in claiming superiority of Kirkwood superposition approximation over WBGA approach since in here it was shown that Kirkwood superposition approximation describes ABBA model qualitatively, but it remains to be seen whether it works on the A+\textit{B} model which WBGA describes well. Similar study (where only single occupancy of lattice sites was allowed and reaction range was assumed short but finite) showed that Kirkwood superposition approximation can describe A+\textit{B} reaction [4], and claim of superposition approximation superiority is likely to be correct but, nevertheless, such claim has to be tested throughly.

The application of Kirkwood superposition approximation to the ABBA and A+B models will be presented in the forthcoming publication as there are many interesting technical details that need to be sorted out. For example, from present study there are some indications (results not shown here) that when using Kirkwood superposition approximation for extremely short range re-
action, such as on-site reaction studied here, care has to be taken so that thermodynamic limit is accounted for properly. It seems that one has to approach Kirkwood superposition approximation through formalism developed in section IV C.

To conclude, it would be interesting to have a relatively simple approximation at hand, not far away from pair approximation, which could be used to extract qualitative asymptotics for arbitrary reaction-diffusion model. Clearly such program is ambitious since in reality one is bound to make approximation which is related to the particular model but, nevertheless, it is worth a try. The A+A and A+B reaction-diffusion models (or combination of them) are excellent bench-mark models and any successful approximation should strive to describe these reactions properly. Present study is a attempt in this direction.

ACKNOWLEDGMENTS

I would like to thank Prof. Malte Henkel and the staff at the Laboratoire de Physique des Materiaux, Universite Henri Poincare Nancy I, for warm hospitality where part of this work was done.

APPENDIX A: APPROXIMATION FOR \( G(t-t') \)

In Eq. (52) sum over \( k \) can be approximated as integral

\[
G(t-t') = \frac{1}{(2\pi)^d} \left[ \int_{-\pi}^{\pi} dpe^{-2Dp^2(t-t')} \right]^d
\]

(A1)

The equality sign is strictly valid in thermodynamic limit only when \( V \to \infty \) has been taken. It is useful to approximate integral above further by changing bounds of integration

\[
G(t-t') \approx \frac{1}{(2\pi)^d} \left[ \int_{-\infty}^{\infty} dpe^{-p^2\Lambda^2-2D\Lambda^2(t-t')} \right]^d
\]

(A2)

\( \Lambda \) corresponds to a large cutoff for the \( k \)-vector summation (it regularizes UV divergences of theory). The comparison of (A1) and (A2) quickly reveal that \( \Lambda \) is a constant roughly equal to \( \pi \). The evaluation of integral above gives Eq. (53) with \( \eta = \frac{1}{2D\Lambda^2} \). It is convenient to chose \( \eta = \frac{1}{8D\Lambda^2} \) and \( \Lambda = 2\sqrt{\pi} \) since this gives correct value for \( G(0) = 1 \). For large \( t-t' \) particular value of \( \Lambda \) appears to be irrelevant, i.e. absent from final expressions for particle density for large times. However, this really depends on the critical dimension of the field theory.

APPENDIX B: INTEGRATION OF SINGULAR KERNEL

In here the numerical treatment of Eqs. (54-55) is described in a more detail. The general procedure for integrating expressions of the type

\[
I_i[f] = \int_0^{t_i} dsK(t_i,s)f(s)
\]

(B1)

where \( K(t,s) \) is singular when \( s \) approaches \( t \) is described in ref. [29]. The \( i = 0, 1, 2, \ldots \) and \( t_i = ih \). In here the particular focus in on the particular form of singular kernel originating from propagator \( G(t,t') \):

\[
K(t,s) = (t-s + \eta)^{-\alpha}
\]

(B2)

The aim is to find quadrature formula which can integrate (B1) exactly if \( f(s) \) is linear within intervals \( t_{i-1}, t_i \). Thus goal is to find coefficients \( w_{ij} \) in

\[
I_i[f] \approx \sum_{j=0}^{i} w_{ij} f(t_j)
\]

(B3)

such that above equation turns equality for piecewise linear function \( f(s) \). Implementing this procedure gives

\[
I_i[f] = \sum_{j=0}^{i+1} \int_{s_j}^{s_{j+1}} dsK(t_i,s)f(s)
\]

(B4)

and after approximating \( f(s) \) as linear function in intervals \( t_j, t_{j+1} \) for \( j = 0, \ldots, i-1 \)

\[
f(s) \approx \frac{s_{j+1}-s}{h} f(s_j) + \frac{s-s_j}{h} f(s_{j+1})
\]

(B5)

gives (B3) with

\[
w_{i0} = \int_0^{s_i} dsK(t_i, s) \frac{h-s}{h}
\]

(B6)

\[
w_{ij} = \int_{s_{j-1}}^{s_j} dsK(t_i, s) \left( \frac{s-s_{j-1}}{h} + \frac{s_{j+1}-s}{h} \right)
\]

(B7)

\[
w_{ii} = \int_{s_{i-1}}^{s_i} dsK(t_i, s) \frac{s-s_{i-1}}{h}
\]

(B8)

and after performing integrals above with \( K(t,s) \) given in (B2)
\[ w_{i0} = \frac{h^{1-\alpha}}{(\alpha - 1)(\alpha - 2)}[(2 - \alpha - i - \eta)(i + \eta)^{1-\alpha} +
+ (i + \eta - 1)^{2-\alpha}] \quad \text{(B9)} \]
\[ w_{ij} = \frac{h^{1-\alpha}}{(\alpha - 1)(\alpha - 2)}[((i - j + \eta - 1)^{2-\alpha} +
+ (i - j + \eta + 1)^{2-\alpha} - 2(i - j + \eta)^{2-\alpha}] \quad \text{(B10)} \]
\[ w_{ii} = \frac{h^{1-\alpha}}{(\alpha - 1)(\alpha - 2)}[\eta^{2-\alpha} +
+ \eta^{2-\alpha}(\alpha - 2)] \quad \text{(B11)} \]

The pair of equations in (54-55) is discretized as follows. First the differential equation (54) is rewritten in integral form as \( n(t) = n_0 - \lambda \int_0^t ds \varphi(s) \) and trapezoidal rule is used to evaluate integral since all functions are well behaved. However, for Eq. (55) the rule (B3) and (B9)-(B11) designed for singular kernel is used. Implementation of this philosophy gives
\[ n_i = n_0 - \lambda h\left[\frac{\varphi_0}{2} + \sum_{j=1}^{i-1} \varphi_j + \frac{\varphi_j}{2}\right] \quad \text{(B12)} \]
\[ \varphi_i = n_i^2 - \lambda \sum_{j=0}^{i-1} u_{ij} \varphi_j - \lambda w_{ii} \varphi_i \quad \text{(B13)} \]

where \( n_i = n(t_i) \) and \( \varphi_i = \varphi(t_i) \) for \( i = 0, 1, 2, \ldots \). Given that all \( n_j \) and \( \varphi_j \) are known for \( j = 0, 1, 2, \ldots, i - 1 \) using equations above it is possible to calculate \( n_i \) and \( \varphi_i \). The iteration is started with \( n_0 = n(0) \) and \( \varphi_0 = \varphi_0 \).

**APPENDIX C: FINDING INVERSE LAPLACE TRANSFORM OF \( \kappa(s) \) FOR \( d = 2 \)**

In here inverse Laplace transform of \( \kappa(s) \) for \( d = 2 \) given in Eq. (98) will be found. Due to the presence of log one has to use Bramovitz contour to perform integration over \( s \). Also, function \( \kappa(s) \) does not have poles. This means that only contribution to \( \kappa(t) \) comes from the branch cut and one obtains
\[ \kappa(t) = 8\pi D \int_0^\infty \frac{du}{u} e^{-ut} \frac{1}{(\gamma_E + \ln(u\eta))^2 + \pi^2} \quad \text{(C1)} \]

It is useful to re-scale integration variable as \( \eta u \to u \) with only change that time variable appears in combination \( \tau \equiv t/\eta \). In the following we set \( \eta = 1 \) but keep in mind that at the end of calculation \( t \) has to be changed into \( t/\eta \).

As \( t \) grows, due to the presence of \( \exp(-ut) \), only smaller and smaller values for \( u \) contribute to the integral above and it is useful to split integration over \( u \) in the two intervals (a) from 0 to \( c \) and (b) from \( c \) to infinity, where \( 0 < c < 1 \); \( \kappa(t) = \kappa_a(t) + \kappa_b(t) \). It is possible to find upper bound for \( \kappa_b \) as follows. Starting from
\[ \kappa_b(t) \leq \frac{8\pi D}{\gamma_E^2 + \pi^2} \int_c^\infty \frac{du}{u} e^{-ut} \quad \text{(C2)} \]

which, upon using the fact that for particular range of integration above \( 1/u \leq 1/c \) and performing remaining integration, gives
\[ \kappa_b(t) \leq \frac{8\pi D}{(\gamma_E^2 + \pi^2)c} e^{-ct} \quad \text{(C3)} \]

It will be shown that \( \kappa_a(t) \) vanishes lot slower than \( \kappa_b(t) \). One can approximate expression for \( \kappa_a \) as
\[ \kappa_a \approx (8\pi D) \int_0^c \frac{du}{u} e^{-ut} \frac{1}{(\ln u)^2} \quad \text{(C4)} \]

and it can be shown that terms omitted do not influence leading order behavior for \( \kappa_a \). By using partial integration expression above becomes
\[ \kappa_a = 8\pi D \left[-t \int_0^c du e^{-ut} \frac{1}{\ln u} + \mathcal{O}(e^{-ct})\right] \quad \text{(C5)} \]

The integral over \( u \) is most conveniently calculated by changing variables \( tu = v \) which gives
\[ \kappa_a(t) \approx \frac{8\pi D}{\ln t} \int_0^{ct} dv e^{-v} \frac{1}{1 - \frac{\ln v}{\ln t}} \quad \text{(C6)} \]

By sending upper integration limit to infinity, and expanding denominator in series over \( \ln v/\ln t \) one gets
\[ \kappa_a = \frac{8\pi D}{\ln t} [1 + \mathcal{O}(1/\ln t)] \quad \text{(C7)} \]

Keeping in mind that transformation \( t \to t/\eta \) has to be made in the expression above gives result for \( \kappa(t) \) in Eq. (99).

[1] A. S. Mikhailov, Phys. Rep. 184, 307 (1989).
[2] V. Privman, “Nonequilibrium Statistical Mechanics in One Dimension”, (Cambridge Univ. Press, 1997)
[3] Comprehensive Chemical Kinetics, Vol. 25, “Diffusion-limited reactions”, C.H. Bamford, C.F.H. Tipper and R.G. Compton Editors, (Elsevier, 1985).
[4] E. Kotomin and V. Kuzovkov, in Comprehensive Chemical Kinetics, Vol. 34, “Modern aspects of diffusion-controlled reactions”, R.G.Compton and G. Hancock Editors, (Elsevier, 1996).
[5] E. Kotomin and V. Kuzovkov, Rep. Prog. Phys. 55, 2079 (1992).
The density decay amplitude for A+A model is independent of λ and n₀ while the one of A+B model depends only on n₀ (given that systems are observed below critical dimension, naturally).

L.M. Delves and J.L. Mohamed, “Computational methods for integral equations”, (Cambridge Univ. Press, 1985).

FIG. 1. The numerical solution of Eqs. (54-55) for d = 1, 1.5, 2.5, 3 (solid lines). The dotted lines indicate asymptotics as given by Eq. (74). Time is given in seconds and particle density n(t) is dimensionless in units of particles per site. Initial density n₀ was set equal to 1, and reaction rate λ = 1 s⁻¹ was used.

19 B.P. Lee, J. Phys. A 27, 2633 (1994).
20 A.A. Lushnikov, Zh. Eksp. Teor. Fiz. 91, 1376 (1986).
21 B.P. Lee and J. Cardy, J. Stat. Phys. 80, 971 (1995).
22 M.G. Rudavets, J. Phys. A 26, 5313 (1993).
23 M. Bramson and J.L. Lebowitz, Phys. Rev. Lett. 62(3), 3276 (2000).
24 For example, one way to prepare system initially is to take given number of particles and distribute them randomly one by one on the lattice. This way of preparation leads to Poisson distribution of particle number at each lattice site. Also, it is clear that preparing system in this way does not lead to correlation among particles. Thus, saying that particles are distributed according to Poisson distribution amounts to saying that there are no correlations among them.
25 The initial state of the system was prepared by allowing for birth and annihilation of particles and waiting long enough to establish stationary state. Once this stationary state was reached, particle birth was ceased and system continued to evolve by annihilation process solely.
26 The inverse Fourier transform of \( \langle a_k a_{-k} \rangle \) is defined as
\[
\langle a_x a_{-x} \rangle = \frac{1}{\sqrt{\Omega}} \sum_{k_1, k_2, k_3} e^{i(k_1 x + k_2 y + k_3 z)} \langle a_{k_1} a_{k_2} a_{k_3} \rangle.
\]
27 For original work on weakly non-ideal Bose gases please see N.N. Bogolybov, Izv. Akad. Nauk SSSR (Ser. Fiz.) 11, 77 (1974), or N.N. Bogoliubov, Lectures on Quantum Statistics, (Gordon and Breach, New York, 1967), p.p. 107-119.
28 Y.B. Zeldovich, A.A. Ovchinnikov, Zh. Eksp. Teor. Fiz. 74(5), 1588 (1978).
29 For a very concise review of Smoluchowski’s approach and WBGA, please see A.A. Ovchinnikov, S.F. Timashev, and A.A. Belyy, “Kinetics of diffusion controlled chemical processes”, (Nova Science, 1989).
30 The density decay amplitude for A+A model is independent of λ and n₀ while the one of A+B model depends only on n₀ (given that systems are observed below critical dimension, naturally).

5. D.C. Mattis and M.L. Glasser, Rev. Mod. Phys. 70(3), 979 (1998).
6. J. Cardy, cond-mat/9607163, “Renormalisation group approach to reaction-diffusion problems”.
7. A.S. Mikhailov and V.V. Yashin, J. Stat. Phys. 38(1/2), 347 (1985).
8. For a very concise review of Smoluchowski's approach and WBGA, please see A.A. Ovchinnikov, S.F. Timashev, and A.A. Belyy, “Kinetics of diffusion controlled chemical processes”, (Nova Science, 1989).
9. S.F. Burlatskii, A.A. Ovchinnikov, K.A. Pronin, Zh. Eksp. Teor. Fiz. 92(2), 625 (1987).
10. M. Bramson and J.L. Lebowitz, Phys. Rev. Lett. 61, 941 (1987).
11. Y.B. Zeldovich, A.A. Ovchinnikov, Zh. Eksp. Teor. Fiz. 74(5), 1588 (1978).
12. M.G. Rudavets, J. Phys. A 26, 5313 (1993).
13. For example, one way to prepare system initially is to take given number of particles and distribute them randomly one by one on the lattice. This way of preparation leads to Poisson distribution of particle number at each lattice site. Also, it is clear that preparing system in this way does not lead to correlation among particles. Thus, saying that particles are distributed according to Poisson distribution amounts to saying that there are no correlations among them.
FIG. 2. The numerical solution of Eqs. (152-156) for $d = 1$ with increasing amount of Kirkwood superposition approximation embedded (dotted, dash-dot and dashed line). Full curve is result of a Monte Carlo simulation (average of 500 runs). Parameters used are $L = 1000$, $n_A(0) = 2$, $n_B(0) = 1$, $\lambda = 1$ and $\delta = 2$. 