Application of Bogolyubov's theory of weakly nonideal Bose gases to the $A+A$, $A+B$, $B+B$ reaction-diffusion system

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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. Here the approximation used by Bogolyubov to study a weakly nonideal Bose gas, referred to as the weakly nonideal Bose gas approximation (WBGA), is applied in the analysis of 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). Two types of WBGA are considered, the simpler WBGA-I and the more complicated WBGA-II. All models are defined on the lattice to facilitate comparison with computer experiment (simulation). It is found that the WBGA describes the $A+B$ reaction well, it reproduces the correct $d/4$ density decay exponent. However, it fails in the case of the $A+A$ reaction and the $ABBA$ model. (To cure the deficiency of WBGA in dealing with the $A+A$ model, a hybrid of the WBGA and Kirkwood superposition approximations is suggested.) It is shown that the WBGA-I is identical to the dressed-tree calculation suggested by Lee [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 the $d/4$ decay exponent. Last, the usage of the small n_0 approximation suggested by Mattis and Glasser [Rev. Mod. Phys. **70**, 979 (1998)] is questioned if used beyond the $A+B$ reaction-diffusion model.

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I. INTRODUCTION

A variety of methods have been used to study diffusion-controlled reactions (see, e.g., Refs. [1–8] for review) ranging from the simplest pairlike or Smoluchowskii approach [9] to more sophisticated methods such as many particle density function formalism [4,5] and field theory [6–8]. Here, we focus on the field theory. The field theory is very attractive since it offers a systematic way to do calculation. However, like in any other theory, one needs approximations to solve the problem. The particular way of making approximate calculations will be analyzed, Bogolyubov's theory of weakly nonideal Bose gases [10], referred to in the following as the weakly nonideal Bose gas approximation (WBGA).

Mapping of the stochastic dynamics to field theory can be carried out for lattice [6] and off-lattice [11,9] models: The dynamics is governed by a second quantized Hamiltonian $H(a,a^{\dagger})$,

$$\frac{\partial}{\partial t}\Psi(t)=-H(a,a^{\dagger})\Psi(t), \tag{1}$$

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

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. The problem is that in the most interesting regime, when the dimension of the system is low, below some critical dimension, the perturbation series diverges due to infrared divergences. The infrared divergences are normally controlled in the framework of the renormalization group (RG) technique. So far, such control exists only in a limited amount of cases, the $A+A$ reaction being the simplest example. Clearly, there is a need to avoid perturbative treatment (together with RG) and look for alternative ways of calculation. Here, the focus is on the WBGA.

In somewhat technical terms, the basic idea behind WBGA is to neglect the products containing three or higher number of annihilation operators having nonzero wave vector in the Hamiltonian. This procedure leads to a closed set of equations for particle density and correlation functions. Solving these equations amounts to resummation of infinite series of an diagrams. In this way WBGA appears as a nonperturbative technique which can be used to control infrared divergences of perturbation series. In the following, we will distinguish between two types of approximations, referred to as WBGA-I and WBGA-II, which result in linear and nonlinear sets of equations of motion, respectively.

The WBGA was used to study reaction-diffusion systems previously [8,9,12–14]. For example, $A+A$ reaction was studied in Ref. [12] and $A+B$ in Refs. [13,14]. These applications of WBGA on diffusion-controlled reactions, focussed on highly nontrivial stationary states, characterized considerable amount of spatial correlations among reactants. Also, decay from such correlated states has been studied [15].

The number of studies that employed the WBGA method is not that large and there is certainly a need to analyze this method of calculation further. This is the reason why WBGA is considered in this work. The first goal of the present work is to examine a very different situation from the one studied previously in Refs. [12–14]. Performance of WBGA will be tested on models which have a trivial stationary state (no particles in the system) but a nontrivial way of approaching such a stationary state. In this work, initial condition is taken to be uncorrelated, Poisson-like [16]. The three models will be used as study cases, (i) the $A+A$, (ii) the $A+B$, and (iii) the $ABBA$ model.

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Both the $A+A$ and $A+B$ models have been studied previously by a variety of methods, and are the natural choice for testing the performance of any approximation scheme. A large list of published work on these two reactions can be found in Ref. [17].

The *ABBA* model was formulated and studied in Refs. [18,19] with RG technique using ϵ expansion, and numerical simulation. The model describes a mixture of the $A+A$, $B+B$, and $A+B$ reactions which occur at the same time. There is a need to understand the model much better, in particular, evaluation of the particle density ratio for *A* and *B* particles is of great importance. The second aim is to approach *ABBA* model, once again, but with a nonperturbative method of calculation.

The paper is organized as follows. In Sec. II the model to be studied is specified in detail, and mapping to the field theory is described. The outcome of this section is a Hamiltonian which describes the most general two-species reaction-diffusion model. In Sec. III equations of motion for density and correlation functions are derived using the WBGA method. In Sec. IV the WBGA approach is used to describe the $A+A$ model, with application of WBGA-I discussed in Sec. IV A, and application of WBGA-II in Sec. IV B. Also in Sec. 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 Sec. V $A+B$ model is studied by using WBGA-I and WBGA-II methods. Finally, the analysis of the most complicated of the three models studied here, the *ABBA* model, is presented in Sec. VI. Working of WBGA-I is analyzed in Sec. VI A and of WBGA-II in Sec. VI B. The step by step merger of the WBGA and Kirkwood superposition approximations is discussed in Sec. VI C. The summary and outline of future work is given in Sec. 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 *ABBA* models will be obtained as special cases. It will be assumed that particles cannot 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 the occupation number of the site where particle jumps to. Apart from diffusing, particles annihilate in pairs. Particle ρ sitting at the lattice site x and particle ν sitting at the site y are assumed to annihilate with rate $\sigma_{xy}^{\rho\nu}$. This is schematically denoted as

$$\rho(x)+\nu(y)\to 0, \tag{2}$$

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 the 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,

$$\frac{d}{dt}P(c,t)=\sum_{c'} W_{c'\to c}P(c',t)-\sum_{c'} W_{c\to c'}P(c,t), \tag{3}$$

where c denotes particular configuration of the system being defined by the set of lattice occupation numbers. The $W_{c\to c'}$ denote transition rate from state c into c', and can be obtained from knowledge of D_A, D_B, and $\sigma_{xy}^{\rho\nu}$.

The master equation (3) 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 the Poisson distribution with averages denoted by $n_{0,A}$ and $n_{0,B}$ for *A* and *B* particles, respectively.

Using standard procedures (e.g., as the ones described in Refs. [6,11,9,20]), Eq. (3) can be translated into a Schrödinger-type equation (1) by using second-quantized Hamiltonian $H=H_{\mathrm{D}}+H_{\mathrm{R}}$ where H_{D} describes diffusion and H_{R} reactions. We find lattice formulation convenient, and in here formalism in Ref. [20] is closely followed, which results in

$$H_{\mathrm{D}}=\sum_x \sum_{e(x)} [D_A a_x^\dagger(a_x-a_e)+D_B b_x^\dagger(b_x-b_e)] \tag{4}$$

and

$$H_{\mathrm{R}}=\frac{1}{2}\sum_{x,y} \sigma_{xy}^{AA}(a_x^\dagger+a_y^\dagger+a_x^\dagger a_y^\dagger)a_x a_y+\frac{1}{2}\sum_{x,y} \sigma_{xy}^{BB}(b_x^\dagger+b_y^\dagger$$
$$+b_x^\dagger b_y^\dagger)b_x b_y+\sum_{x,y} \sigma_{xy}^{AB}(a_x^\dagger+b_y^\dagger+a_x^\dagger b_y^\dagger)a_x b_y. \tag{5}$$

$a_x^\dagger$, a_x, $b_x^\dagger$, and b_x are creation and annihilation operators for *A* and *B* particles, respectively;

$$[a_x,a_y^\dagger]=\delta_{x,y},\quad [b_x,b_y^\dagger]=\delta_{x,y},$$
$$[a_x,b_y^\dagger]=[a_x^\dagger,b_y]=0, \tag{6}$$

and $[\mathrm{I},\mathrm{II}]\equiv \mathrm{III}-\mathrm{III}$ denotes commutator. The observables can be calculated as

$$\langle O[n_x(t)]\rangle=\langle 0|O[(a_x^\dagger+1)a_x]e^{-Ht}|\Psi_0\rangle, \tag{7}$$

where $O(n_x)$ denotes any function which depends on particle numbers in an arbitrary way. Appearance of $a_x^\dagger+1$ in the right-hand side of Eq. (7), instead of expected $a_x^\dagger$, has to do with the fact that bra-vector $\langle 0|$ is true vacuum state. This point is nicely discussed in Ref. [6]. The generalization of Eq. (7) to more complicated form for $O(n_x,n_y,\ldots)$ is trivial. The Ψ_0 is given by

$$\Psi_0=\exp\left[n_{0,A}\sum_x a_x^\dagger+n_{0,B}\sum_x b_x^\dagger\right]|0\rangle. \tag{8}$$

In the following we compactify notation and use

$$\langle f(a_x,a_y^\dagger,\ldots)\rangle \equiv \langle 0|f(a_x,a_y^\dagger,\ldots)e^{-Ht}|\Psi_0\rangle, \quad (9)$$

where f denotes any function of operators a_x, $a_y^\dagger$, b_x, and $b_y^\dagger$ for any x and y.

To avoid effects of boundaries periodic boundary conditions are assumed and one can introduce Fourier transforms for operators,

$$a_x=\frac{1}{\sqrt{V}}\sum_k e^{ikx}a_k, \quad a_x^\dagger=\frac{1}{\sqrt{V}}\sum_k e^{-ikx}a_k^\dagger, \quad (10)$$

$$b_x=\frac{1}{\sqrt{V}}\sum_k e^{ikx}b_k, \quad b_x^\dagger=\frac{1}{\sqrt{V}}\sum_k e^{-ikx}b_k^\dagger \quad (11)$$

and reaction rates

$$\sigma_x^{\rho\nu}=\frac{1}{V}\sum_k \sigma_k^{\rho\nu}e^{ikx}, \quad \sigma_k^{\rho\nu}=\sum_x \sigma_x^{\rho\nu}e^{-ikx} \quad (12)$$

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 H in terms of creation and annihilation operators in k space. Starting from Eqs. (4) and (5), and using Eqs. (10)–(12) gives

$$H_{\mathrm{D}}=D_A\sum_k k^2a_k^\dagger a_k+D_B\sum_k k^2b_k^\dagger b_k+O(k^4) \quad (13)$$

and

$$\begin{aligned}H_{\mathrm{R}}=&\frac{1}{\sqrt{V}}\sum_{q,k}\sigma_q^{AA}a_k^\dagger a_{k-q}a_q+\frac{1}{2V}\sum_{q,k,l}\sigma_q^{AA}a_k^\dagger a_l^\dagger a_{k-q}a_{l+q}\\&+\frac{1}{\sqrt{V}}\sum_{q,k}\sigma_q^{BB}b_k^\dagger b_{k-q}b_q+\frac{1}{2V}\sum_{q,k,l}\sigma_q^{BB}b_k^\dagger b_l^\dagger b_{k-q}b_{l+q}\\&+\frac{1}{\sqrt{V}}\sum_{q,k}\sigma_q^{AB}(a_k^\dagger a_{k-q}b_q+b_k^\dagger b_{k-q}a_q)\\&+\frac{1}{V}\sum_{q,k,l}\sigma_q^{AB}a_k^\dagger b_l^\dagger a_{k-q}b_{l+q}.\end{aligned} \quad (14)$$

Please note that Eq. (13) is an approximation which is valid for small k. The form in Eq. (14) is exact. Once the explicit form of H is known, one can proceed with calculation of particle density, as shown in the following section.

III. EQUATIONS OF MOTION FOR DENSITY AND THE CORRELATION FUNCTIONS

Equation (7) 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 $O=a_x^\dagger a_x$ and $O=b_x^\dagger b_x$, respectively; using Eq. (7) one gets $n_A(x,t)=\langle a_x\rangle$ and $n_B(x,t)=\langle b_x\rangle$. Furthermore, if initial conditions are translationally invariant, which is the case for Poisson-distributed particles, one has

$$n_A(t)\equiv\frac{1}{V}\left\langle\sum_x a_x\right\rangle=\frac{1}{\sqrt{V}}\langle a_0\rangle, \quad (15)$$

$$n_B(t)\equiv\frac{1}{V}\left\langle\sum_x b_x\right\rangle=\frac{1}{\sqrt{V}}\langle b_0\rangle, \quad (16)$$

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

The time derivative of $n_A(t)$ and $n_B(t)$ is controlled by $[a_0,H]$ and $[b_0,H]$, respectively. Evaluating commutators gives equations of motion,

$$\frac{\partial n_A}{\partial t}=-\left[\sigma_0^{AA}n_An_A+\sigma_0^{AB}n_An_B+\frac{1}{V}\sum_{k\neq 0}(\sigma_k^{AA}\Gamma_k^{AA}+\sigma_k^{AB}\Gamma_k^{AB})\right], \quad (17)$$

$$\frac{\partial n_B}{\partial t}=-\left[\sigma_0^{BB}n_Bn_B+\sigma_0^{AB}n_An_B+\frac{1}{V}\sum_{k\neq 0}(\sigma_k^{BB}\Gamma_k^{BB}+\sigma_k^{AB}\Gamma_k^{AB})\right], \quad (18)$$

where

$$\Gamma_k^{AA}\equiv\langle a_ka_{-k}\rangle, \quad \Gamma_k^{BB}\equiv\langle b_kb_{-k}\rangle, \quad \Gamma_k^{AB}\equiv\langle a_kb_{-k}\rangle. \quad (19)$$

To derive Eqs. (17) and (18) the sum over k is split into $k=0$ and $k\neq 0$ parts and assumption is made that $k=0$ components are nonfluctuating, i.e., $\langle a_0a_0\rangle\approx\langle a_0\rangle\langle a_0\rangle$ and likewise for $\langle a_0b_0\rangle$ and $\langle b_0b_0\rangle$ (thermodynamic limit).

Equations (17) and (18) involve correlation functions $\Gamma_k^{\rho\nu}$ with $\rho,\nu=A,B$. Again, evaluation of $[O,H]$ with $O=a_ka_{-k}$, a_kb_{-k}, b_kb_{-k} gives

$$\frac{\partial}{\partial t}\Gamma_k^{AA}=-2D_Ak^2\Gamma_k^{AA}-\left[\sigma_k^{AA}n_A^2+\frac{1}{V}\sum_{q\neq k}\sigma_q^{AA}\Gamma_{k-q}^{AA}+2(\sigma_0^{AA}+\sigma_k^{AA})n_A\Gamma_k^{AA}+\sigma_k^{AB}n_A(\Gamma_k^{AB}+\Gamma_{-k}^{AB})+2\sigma_0^{AB}n_B\Gamma_k^{AA}\right], \quad (20)$$

$$\frac{\partial}{\partial t}\Gamma_k^{BB}=-2D_Bk^2\Gamma_k^{BB}-\left[\sigma_k^{BB}n_B^2+\frac{1}{V}\sum_{q\neq k}\sigma_q^{BB}\Gamma_{k-q}^{BB}+2(\sigma_0^{BB}+\sigma_k^{BB})n_B\Gamma_k^{BB}+\sigma_k^{AB}n_B(\Gamma_k^{AB}+\Gamma_{-k}^{AB})+2\sigma_0^{AB}n_A\Gamma_k^{BB}\right], \quad (21)$$

$$\frac{\partial}{\partial t}\Gamma_k^{AB} = -(D_A+D_B)k^2\Gamma_k^{AB} - \left[\sigma_k^{AB} n_A n_B + \frac{1}{V}\sum_{q\neq k}\sigma_q^{AB}\Gamma_{k-q}^{AB}\right] - [(\sigma_0^{AA}+\sigma_k^{AA})n_A + (\sigma_0^{BB}+\sigma_k^{BB})n_B + \sigma_0^{AB}(n_A+n_B)]\Gamma_k^{AB} - \sigma_k^{AB}(n_A\Gamma_k^{BB}+n_B\Gamma_k^{AA}). \quad (22)$$

Equations (20), (21), and (22) 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.

A few comments about the inversion symmetry (in k space) of $\Gamma_k^{\rho\nu}$ $\rho,\mu=A,B$ are in order. By construction, $\Gamma_k^{\rho\rho}(t)=\Gamma_{-k}^{\rho\rho}(t)$ for $\rho=A,B$ since these functions represent correlations for same operator types. It can be checked that the same property holds for Γ_k^{AB}, provided it is true at $t=0$. This is indeed the case since the initial conditions for $\Gamma_k^{\rho\nu}$ with $\rho\nu=A,B$ are given by

$$\Gamma_k^{\rho\nu}(0)=\Delta_{k,0}Vn_{0,\rho}n_{0,\nu}, \quad \rho,\nu=A,B, \quad (23)$$

where $\Delta_{x,y}$ denotes Kronecker delta function,

$$\Delta_{x,y}=\begin{cases}1, & x=y\\ 0, & x\neq y.\end{cases} \quad (24)$$

In the following, whenever $\Gamma_k^{AB}+\Gamma_{-k}^{AB}$ appears in the equations of motion, we will use the assumption of inversion symmetry and shorten the expression to $2\Gamma_k^{AB}$.

The last terms in Eqs. (20)–(22), which are products of density and correlator, and appear to be third order in density $O(n^3)$, lead to nonlinear equations of motion. These terms come from averages of the type $\langle a_k a_q a_l\rangle$ where one of the $\{k,q,l\}$ momenta is zero while remaining two are not. Being third order in density, it is tempting to neglect these terms. To test the effect of neglecting or keeping $\mathcal{O}(n^3)$ terms two approximations will be studied, WBGA-I and 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. 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 Eqs. (17)–(18) and (20)–(22). To obtain equations of motion for the $ABBA$ model one simply sets $D_A=D_B=D$ and

$$\sigma_{xy}^{AA}=\sigma_{xy}^{BB}=\lambda\Delta_{x,y}, \quad \sigma_{xy}^{AB}=\delta\Delta_{x,y}. \quad (25)$$

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 Eq. (25) with $\delta=0$ in Eqs. (17)–(18) and (20)-(22) gives equation of motion for the density

$$\frac{\partial n}{\partial t}=-\lambda[n^2+\Phi] \quad (26)$$

and the correlator

$$\frac{\partial}{\partial t}\Gamma_k=-2Dk^2\Gamma_k-\lambda[n^2+\Phi]-4\lambda n\Gamma_k. \quad (27)$$

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

$$\Phi(t)=\frac{1}{V}\sum_{k\neq 0}\Gamma_k(t). \quad (28)$$

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. WBGA-I

In the WBGA-I, when term proportional to $n\Gamma_k$ is dropped, Eq. (27) can be studied analytically. Uncorrelated (Poisson-like) initial condition is described by $\Gamma_k(0)=\delta_{k,0}Vn_0^2$ and solution of Eq. (27), with $k\neq 0$, reads

$$\Gamma_k(t)=-\lambda\int_0^t dt' e^{-2Dk^2(t-t')}[n(t')^2+\Phi(t')]. \quad (29)$$

Please note that the $\Gamma_0(t)$ is determined from $\Gamma_0(t)=Vn(t)^2$ (thermodynamic limit) and not from Eq. (29). Summation of Eq. (29) over $k\neq 0$ and division by V gives

$$\Phi(t)=-\lambda\int_0^t dt' G(t-t')[n(t')^2+\Phi(t')], \quad (30)$$

where

$$G(t-t')\equiv\frac{1}{V}\sum_{k\neq 0}e^{-2k^2D(t-t')} \quad (31)$$

was introduced. For large lattice size when $V\to\infty$, expression above can be approximated as

$$G(t-t')\approx[8\pi D(t-t'+\eta)]^{-d/2}, \quad (32)$$

where $\eta=1/8\pi D$.

Equations (26), (30), and (32) 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. (26) and (30) as

$$\frac{\partial n}{\partial t}=-\lambda\varphi, \quad (33)$$

$$\varphi(t)=n(t)^2-\lambda\int_0^t dt' G(t-t')\varphi(t'), \tag{34}$$

which completely specify $n(t)$. Equations (33) and (34) have been analyzed in the entirely different context of $A+B$ reaction in Ref. [6] where it was shown that asymptotic density decay is given by

$$n(t)\sim\sqrt{n_0}(8\pi Dt)^{-d/4}. \tag{35}$$

There is another way of extracting asymptotics which is interesting to look at. By using Laplace transform it is possible to transform Eqs. (33) and (34) into a single equation. Laplace transform is defined as

$$X(s)=\int_0^\infty dt e^{-st}X(t). \tag{36}$$

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. (34) one gets $\varphi(s)=n_2(s)-\lambda g(s)\varphi(s)$, and combining it with $\varphi(s)=(sn(s)-n_0)/\lambda$ from Eq. (33) gives

$$n_2(s)=\left[g(s)+\frac{1}{\lambda}\right][n_0-sn(s)]. \tag{37}$$

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

$$g(s)=(8\pi D)^{-d/2}e^{\eta s}s^{d/2-1}\Gamma(1-d/2,\eta s). \tag{38}$$

$\Gamma(\beta,x)$ denotes the incomplete gamma function,

$$\Gamma(\beta,x)=\int_x^\infty du\, u^{-1+\beta}e^{-u}. \tag{39}$$

The analytic continuation of $\Gamma(\beta,x)$ is possible. For noninteger β 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. (37) results in

$$sn(s)-n_0=-\lambda_{\rm eff}(s)n_2(s), \tag{40}$$

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

$$\lambda_{\rm eff}(s)=\frac{\lambda}{1+\lambda g(s)}. \tag{41}$$

Finally, taking the inverse Laplace transform of Eq. (40) gives

$$\frac{\partial n}{\partial t}=-\int_0^t dt'\lambda_{\rm eff}(t-t')n(t')^2. \tag{42}$$

Equation (42) was obtained in Ref. [20], in the context of $A+A$ reaction, through a diagrammatic technique and referred to as the *dressed-tree* calculation. Thus here we have shown that WBGA-I is equivalent to the dressed-tree calculation. Also, the following solution to Eq. (42) was suggested [21]:

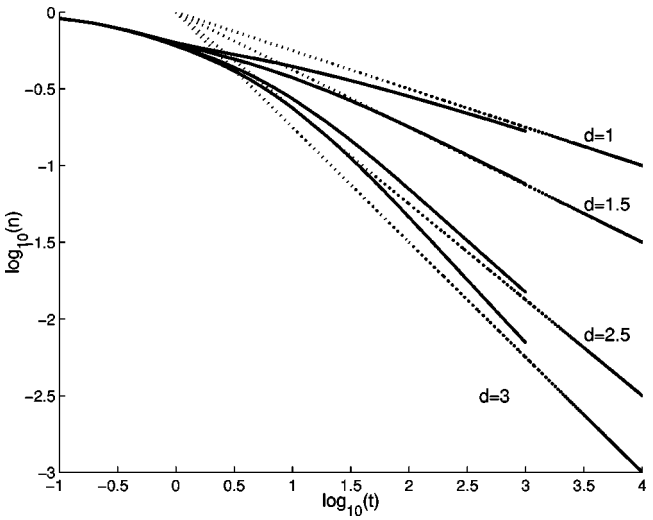

FIG. 1. The numerical solution of Eqs. (33) and (34) for $d=1$, 1.5, 2.5, 3 (solid lines). The dotted lines indicate asymptotics as given by Eq. (35). Time is given in seconds and particle density $n(t)$ is dimensionless in units of particles per site. Initial density n_0 was set equal to 1, and reaction rate $\lambda=1\ \mathrm{s}^{-1}$ was used.

$$n(t)\sim-\frac{\Gamma(1-d/2)^2}{\Gamma(1-d)}(8\pi Dt)^{-d/2}. \tag{43}$$

However, Eqs. (33)–(34) and Eq. (42) are fully equivalent and expressions in Eqs. (35) and (43) should be the same. Clearly, studies [20] and [6] suggest contradictory results: Ref. [20] argues that the dressed-tree calculation gives $d/2$ decay exponent for particle density, while Ref. [6] argues for the $d/4$ decay exponent. Solution to this paradox is discussed in Appendix A where analysis of Ref. [20] is repeated. It is shown that in Ref. [20] 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. (42).

Thus the first main finding of this section is that WBGA-I predicts wrong density decay exponent for $A+A$ reaction. It gives exponent value of $d/4$ instead of $d/2$. The second finding is that the dressed-tree calculation suggested in Ref. [20] is equivalent to WBGA-I (and fails to describe $A+A$ reaction).

Figure 1 offers graphical representation of these results. The numerical treatment of Eqs. (33) and (34) confirms the asymptotic decay given in Eq. (35). Equations (33) and (34) 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 a concave form (bent upward), while curves in Fig. 1 of Ref. [6] are convex (bent 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

differences could come from the numerical treatment. The details of numerical treatment used in this work are shown in Appendix B.

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

B. WBGA-II

When term $n\Gamma_k$ is kept in Eq. (27), equivalent of Eq. (34) reads

$$\varphi(t)=n(t)^2-\lambda\int_0^t dt' I(t,t')\varphi(t'), \tag{44}$$

while Eq. (33) stays the same. The $I(t,t')$ is given by

$$I(t,t')=G(t-t')\exp\left[-4\lambda\int_{t'}^t dt'' n(t'')\right]. \tag{45}$$

The asymptotics of Eq. (44) cannot be extracted by Laplace transform, and it is more convenient to use the approach of Ref. [6]. For large t, Eq. (44) can be approximated by

$$\varphi(t)\approx n(t)^2-I(t,0)\mathcal{I}(t), \tag{46}$$

where $\mathcal{I}(t)\equiv\lambda\int_0^t dt'\varphi(t')$. This step is valid provided two conditions are satisfied. First, the term $I(t,t')$ has to vanish as time difference $t-t'$ grows. Second, the integral $\int_0^\infty dt\varphi(t)$ has to be finite. Using Eq. (33) one gets $\mathcal{I}(t)=n_0-n(t)\approx n_0$ and Eq. (46) becomes

$$\frac{\partial n}{\partial t}\approx-\lambda n^2+\lambda I(t,0)n_0. \tag{47}$$

The equation above is solved with the assumption that asymptotically $n(t)\sim\mathcal{A}/t$, which is checked self-consistently at the end. Using postulated asymptotics for t, one can see from Eq. (45) that $I(t,0)\sim\text{const}\times t^{-(d/2+4\lambda\mathcal{A})}$. Assuming that

$$\frac{I(t,0)}{n(t)^2}\to 0,\quad t\to\infty, \tag{48}$$

one can solve Eq. (47) in the form $\partial n/\partial t=-\lambda n^2$, and get $\mathcal{A}=1/\lambda$. Assumption (48) is correct provided $2<d/2+4\lambda\mathcal{A}=d/2+4$, which is true for any d. This shows that $n(t)\approx 1/(\lambda t)$ is the asymptotic form for the solution of Eqs. (33) and (44). This means that the last term $(n\Gamma_k)$ in Eq. (27) 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 the $A+A$ reaction. This is somewhat surprising as even the simplest pair approach, e.g. Smoluchowskii method, describes the exponent of $A+A$ correctly. Clearly $A+A$ reaction cannot 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 following subsection.

C. The hybrid of the WBGA and Kirkwood superposition approximation (WBGA/Kirkwood)

To see how to improve the WBGA one has to clarify what went wrong in the first place. We start from the problematic equation Eq. (20) which becomes (27) when terms with σ_k^{AB} are set to zero. To trace why the WBGA fails it is useful to rewrite Eq. (20) as it looks one step before the WBGA is made, and we keep only terms describing $A+A$ reaction:

$$\frac{\partial}{\partial t}\Gamma_k=-2Dk^2\Gamma_k-\left[\sigma_k n^2+\frac{1}{V}\sum_{q\neq k}\sigma_q\Gamma_{k-q}\right]-\dot{\Gamma}^{(3)}, \tag{49}$$

where

$$\dot{\Gamma}^{(3)}=\frac{1}{\sqrt{V}}\sum_q\sigma_q(\langle a_{-k}a_{k-q}a_q\rangle+\langle a_k a_{-k-q}a_q\rangle) \tag{50}$$

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

$$\langle a_{k_1}a_{k_2}a_{k_3}\rangle=\langle a_x a_y a_z\rangle=0, \tag{51}$$

while in WBGA-II one assumes

$$\begin{aligned}\langle a_{k_1}a_{k_2}a_{k_3}\rangle\approx{}&\Delta_{k_1,0}\Delta_{k_2,0}\Delta_{k_3,0}a_0^3+\Delta_{k_1,0}\overline{\Delta}_{k_2,0}\overline{\Delta}_{k_3,0}a_0\langle a_{k_2}a_{k_3}\rangle\\&+\overline{\Delta}_{k_1,0}\Delta_{k_2,0}\overline{\Delta}_{k_3,0}a_0\langle a_{k_1}a_{k_3}\rangle\\&+\overline{\Delta}_{k_1,0}\overline{\Delta}_{k_2,0}\Delta_{k_3,0}a_0\langle a_{k_1}a_{k_2}\rangle,\end{aligned} \tag{52}$$

where the notation $\overline{\Delta}_{k,q}=1-\Delta_{k,q}$ was introduced. Inserting Eq. (52) into Eq. (49) gives the terms describing $A+A$ process in Eq. (20). It is useful to transform the approximation above into the x space to understand the nature of approximation better. The inverse Fourier transform of Eq. (52) gives [22]

$$\begin{aligned}\langle a_x a_y a_z\rangle\approx{}&n^3+n(\langle a_x a_y\rangle-n^2)+n(\langle a_x a_z\rangle-n^2)\\&+n(\langle a_y a_z\rangle-n^2).\end{aligned} \tag{53}$$

By looking at Eq. (53) it is possible to understand why the WBGA fails in the case of $A+A$ reaction. Equation (53) suggests that the WBGA is somewhat equivalent to the additive expansion of correlation functions. It has been argued that such an additive approximation is inferior to the Kirkwood superposition approximation [4,5], and analysis was done for fermionic models, but is likely to be valid for bosonic models as well (at least for the ones considered here). Clearly, to correctly describe $A+A$ reaction one has to use Kirkwood superposition approximation. How can one implement such an approximation for bosonic models?

The usage of the Kirkwood superposition approximation in the context of reaction-diffusion models has been thoroughly tested in the case of fermionic representation, where double occupancy of lattice sites is not allowed (for a nice review see, e.g., Ref. [4]). In such a case the Kirkwood superposition approximation is expressed through

$$\langle n_x n_y n_z\rangle \approx \langle n_x n_y\rangle\langle n_x n_z\rangle\langle n_y n_z\rangle/n^3, \tag{54}$$

and it was shown that the correct $d/2$ density decay exponent results from this procedure. However, when multiple occupancy of lattice sites is allowed, as is done here, one has to be careful. Another way of carrying out the Kirkwood superposition approximation would be to take

$$\langle a_x a_y a_z\rangle \approx \frac{1}{n^3}\langle a_x a_y\rangle\langle a_x a_z\rangle\langle a_y a_z\rangle. \tag{55}$$

In the case of fermionic representation there is no ambiguity whether to use Eq. (54) or Eq. (55) as they are fully equivalent, owing to the fact that field theoretic averages of type $\langle n_x n_x\rangle$ are not possible in fermionic representation, however, they are bosonic where a choice between Eqs. (54) and (55) has to be made.

By studying Eqs. (54) and (55) around $t=0$ it is possible to see that approximation (55) is more reasonable one. Such an analysis is omitted to save the space. Thus, in here, we argue that Eq. (55) is a more reasonable platform for carrying out the Kirkwood superposition approximation in the case of bosonic field theory. Also, for on-site reaction model as studied here, it is crucial that averages of the type $\langle a_x a_x\rangle$ are treated correctly. Therefore, in the following, Eq. (55) will not be used directly, but will be modified further in the spirit of the WBGA, accounting for the thermodynamic limit.

The Kirkwood superposition approximation in Eq. (55) is rephrased in the k space which gives [23]

$$\langle a_{k_1} a_{k_2} a_{k_3}\rangle \approx \frac{\delta(k_1+k_2+k_3)}{n^3 V^{3/2}} \sum_l \Gamma_l \Gamma_{k_1-l}\Gamma_{k_2+l}. \tag{56}$$

To get the improved form for three body terms one inserts Eq. (56) into Eq. (50), leading to

$$\dot{\Gamma}^{(3)} \approx \frac{2}{n^3 V^2} \sum_{q,l} \sigma_q \Gamma_l \Gamma_{k+l}\Gamma_{k-q+l}. \tag{57}$$

The expression above was obtained by using symmetry properties $\Gamma_k=\Gamma_{-k}$ and $\sigma_q=\sigma_{-q}$. Also, upon inserting Eq. (56) into Eq. (50), the two terms on the right-hand side of Eq. (50) contribute equally resulting in factor 2 in Eq. (57).

In the spirit of WBGA the terms in Eq. (56) which contain large number of correlation functions with k vector different from zero are neglected. Also, care is taken to account for the thermodynamic limit, where $k=0$ components are treated separately. 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 the sums various contributions from sum over l are distilled to extract nonfluctuating $k=0$ operators. This gives

$$\dot{\Gamma}^{(3)} \approx \frac{2}{n^3 V^2}\Big[\sigma_k(\Gamma_0^2\Gamma_k+\Gamma_0\Gamma_k^2) + \sum_{q\neq k} \sigma_q\Gamma_0(\Gamma_k\Gamma_q+\Gamma_k\Gamma_{k-q}+\Gamma_q\Gamma_{q-k})\Big], \tag{58}$$

where terms of the type $\Gamma_k\Gamma_q\Gamma_l$ with $k,q,l\neq 0$ have been neglected.

The first term on the right-hand side of Eq. (58) can be neglected since it leads to mean field behavior (as shown in Sec. IV B). The second term can be absorbed into 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 nontrivial way and are neglected in the following for simplicity reasons. With $\Gamma_0 \approx n^2 V$, and applying the recipe just described gives

$$\dot{\Gamma}^{(3)} \approx \frac{2}{n}\Gamma_k\left(\sigma_0 n^2 + \frac{1}{V}\sum_{q\neq 0}\sigma_q\Gamma_q\right), \tag{59}$$

which is midway between the WBGA-II [Eq. (52)] and Kirkwood superposition approximation [Eq. (56)]. It is interesting to contrast the equation above with the shortened Kirkwood superposition approximation discussed in Refs. [4,5] in the context of fermionic models. There is some similarity, but descriptions are far from being identical.

Using approximation (59), referred to in the following as the WBGA/Kirkwood approximation, to decouple three body density, and a particular form for σ_{xy}^{AA} used throughout this section, gives equations of motion

$$\frac{\partial}{\partial t}\Gamma_k = -2Dk^2\Gamma_k - \lambda(n^2+\Phi) - 2\lambda\Gamma_k\frac{\Phi+n^2}{n}, \tag{60}$$

which should be contrasted with Eq. (27). The most convenient way to solve Eqs. (26) and (60) is to introduce χ_k as $\Gamma_k=n^2\chi_k$ and $n^2+\Phi=n^2\chi$ where $\chi\equiv 1+(1/V)\Sigma_{k\neq 0}\chi_k$, and χ_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. (26) into

$$\frac{\partial}{\partial t}n(t) = -\kappa(t)n(t)^2, \tag{61}$$

where effective reaction rate $\kappa(t)=\lambda\chi(t)$ was introduced. Same change of variables transforms Eq. (60) into

$$\frac{\partial}{\partial t}\chi_k = -2Dk^2\chi_k - \lambda\chi. \tag{62}$$

Equation (62) can be solved for all χ_k and $k\neq 0$ [pretending that $\chi(t)$ is known], and after summing over $k\neq 0$ one gets the following integral equation:

$$\chi(t) = 1-\lambda\int_0^t dt' G(t-t')\chi(t'). \tag{63}$$

The solution of the equation above can be found by a Laplace transform which gives

$$\kappa(s)=\frac{\lambda}{s[1+\lambda g(s)]}. \tag{64}$$

Also, one can integrate Eq. (61), which gives

$$n(t)=\frac{n_0}{1+n_0\overline{\kappa}(t)}, \quad \overline{\kappa}(t)=\int_0^t dt'\,\kappa(t'). \tag{65}$$

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

Inserting small s expansion of $g(s)$ [see Eqs. (A4) and (A5)] into Eq. (64) gives

$$\kappa(s)\sim\begin{cases}\dfrac{(8\pi D)^{d/2}}{\Gamma(1-d/2)}s^{-d/2}, & d<2\\ -\dfrac{8\pi D}{s[\gamma_E+\ln(\eta s)]}, & d=2\\ \dfrac{\lambda}{1+\lambda g(0)}s^{-1}, & d>2\end{cases} \tag{66}$$

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

$$\kappa(t)\sim\begin{cases}\dfrac{(8\pi D)^{d/2}}{\Gamma(1-d/2)\Gamma(d/2)}t^{d/2-1}, & d<2\\ \dfrac{8\pi D}{\ln t/\eta}, & d=2\\ \dfrac{\lambda}{1+\lambda g(0)}, & d>2\end{cases} \tag{67}$$

when $t\to\infty$. To find the inverse Laplace transform of $\kappa(s)$ for $d=2$ [second line of Eq. (66)] is somewhat involved; please see Appendix C for details. Finally, inserting Eq. (67) into Eq. (65) gives the following asymptotics:

$$n(t)\sim\begin{cases}\Gamma(1-d/2)\Gamma(1+d/2)(8\pi Dt)^{-d/2}, & d<2\\ \dfrac{\ln 8\pi Dt}{8\pi Dt}, & d=2\\ \left[\dfrac{1}{\lambda}+g(0)\right]t^{-1}, & d>2,\end{cases} \tag{68}$$

where $g(0)$ entering in the third row can easily be found from Eq. (A4). Thus, in here, it was shown that Kirkwood superposition approximation reproduces correct density decay exponent $d/2$ when implemented following Eq. (55).

V. WBGA APPLIED TO THE $A+B$ REACTION

Equations of motion for density and correlation functions describing the $A+B$ model result from Eqs. (17) and (18) and Eqs. (20)–(22) by using Eq. (25) with $\lambda=0$. For simplicity, we focus on $n_A=n_B\equiv n$ case and omit labels A and B. Also, as in the preceding section $n_0=n_{0,A}=n_{0,B}$. Applying the procedure outlined above leads to the equations for particle densities

$$\frac{\partial n}{\partial t}=-\delta(n^2+\Phi_c), \tag{69}$$

where Φ_c is given by the AB correlation function,

$$\Phi_c(t)=\frac{1}{V}\sum_{k\neq 0}\Gamma_k^{AB}(t). \tag{70}$$

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

$$\left(\frac{\partial}{\partial t}+2Dk^2\right)\Gamma_k^c=-\delta(n^2+\Phi_c)-2\delta n(\Gamma_k+\Gamma_k^c), \tag{71}$$

$$\left(\frac{\partial}{\partial t}+2Dk^2\right)\Gamma_k=-2\delta n(\Gamma_k+\Gamma_k^c). \tag{72}$$

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

$$\Phi_c(t)=-\delta\int_0^t dt'[G(t,t')+I(t,t')][n(t')^2+\Phi_c(t')] \tag{73}$$

and for AA (or BB) pairs as

$$\Phi(t)=\delta\int_0^t dt'[G(t,t')-I(t,t')][n(t')^2+\Phi_c(t')]. \tag{74}$$

The $I(t,t')$ appearing in Eqs. (73) and (74) has the same form as in Eq. (45) with trivial change of λ into δ. The same type of analysis as in Sec. IV B leads to the 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 the correct $d/4$ exponent when used to solve the $A+B$ model.

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

VI. WBGA APPLIED TO THE $ABBA$ MODEL

The $ABBA$ model was suggested in Refs. [18,19]. The mean field analysis of this model predicts that minority species has to die out asymptotically, $u(t)\equiv n_B(t)/n_A(t)\to 0$ as $t\to\infty$, minority species being the one with smaller concentration at $t=0$. (For convenience we chose B species to be minority, $n_{0,A}>n_{0,B}$.) However, fluctuations lead to quite remarkable survival of minority species. Below critical dimension $u(t)\to$const (provided $D_A=D_B$, for $D_A\neq D_B$ one of the species dies out [24]).

There are two reasons for studying $ABBA$ model here.

First, the calculation of the asymptotic particle density ratio is still an open question. The previously used ϵ-expansion technique could not reveal the form of $u(\infty)$. $u(\infty)$ has an interesting property that it depends both on reaction rates and initial particle concentrations, while individual reactions do not [25]. Thus, in here, calculation of $u(\infty)$ is attempted again, with a different calculation scheme, the WBGA method. Second, the $A+A$ and $A+B$ reactions have been studied in previous sections but now they are allowed to occur simultaneously. It is interesting to see how the WBGA approach performs in such a situation.

We start from equations of motion given in Sec. III which describe a very general two species reaction-diffusion model. Assumptions in Eq. (25) describe the content of the *ABBA* model. Using Eq. (25) in Eqs. (17) and (18) gives

$$\frac{\partial}{\partial t}n_A = -(\lambda n_A^2 + \delta n_A n_B + \lambda \Phi_{AA} + \delta \Phi_{AB}), \tag{75}$$

$$\frac{\partial}{\partial t}n_B = -(\lambda n_B^2 + \delta n_A n_B + \lambda \Phi_{BB} + \delta \Phi_{AB}), \tag{76}$$

where

$$\Phi_{\rho\nu} = \frac{1}{V}\sum_{k\neq 0}\Gamma_k^{\rho\nu}, \quad \rho,\nu = A,B. \tag{77}$$

Also, equations for correlators (20)–(22) simplify to

$$\frac{\partial}{\partial t}\Gamma_k^{AA} = -2Dk^2\Gamma_k^{AA} - \lambda(n_A^2 + \Phi_{AA}) - 2(2\lambda n_A + \delta n_B)\Gamma_k^{AA} - 2\delta n_A \Gamma_k^{AB}, \tag{78}$$

$$\frac{\partial}{\partial t}\Gamma_k^{BB} = -2Dk^2\Gamma_k^{BB} - \lambda(n_B^2 + \Phi_{BB}) - 2(2\lambda n_B + \delta n_A)\Gamma_k^{BB} - 2\delta n_B \Gamma_k^{AB}, \tag{79}$$

$$\frac{\partial}{\partial t}\Gamma_k^{AB} = -2Dk^2\Gamma_k^{AB} - \delta(n_A n_B + \Phi_{AB}) - (2\lambda + \delta)(n_A + n_B)\Gamma_k^{AB} - \delta(n_A\Gamma_k^{BB} + n_B\Gamma_k^{AA}). \tag{80}$$

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

A. WBGA-I

In the framework of WBGA-I all seemingly $O(n^3)$ terms of the type $n_\rho\Gamma_k^\nu$ with $\rho = A,B$ and $\nu = AA,AB,BB$ are thrown away in Eqs. (78)–(80). Following steps, similar to those of Sec. IV A, gives

$$\frac{\partial}{\partial t}n_A = -(\lambda\varphi_{AA} + \delta\varphi_{AB}), \tag{81}$$

$$\frac{\partial}{\partial t}n_B = -(\lambda\varphi_{BB} + \delta\varphi_{AB}) \tag{82}$$

and

$$\varphi_{\rho\nu} \equiv n_\rho n_\nu - \Lambda_{\rho\nu}\int_0^t dt' G(t-t')\varphi_{\rho\nu}(t'),$$

$$\Lambda_{\rho\nu} \equiv (\lambda\Delta_{\rho,\nu} + \delta\overline{\Delta}_{\rho,\nu}),$$

$$\varphi_{\rho\nu} \equiv n_\rho n_\nu + \Phi_{\rho\nu} \tag{83}$$

for $\rho,\nu \in \{A,B\}$. To solve Eqs. (81)–(83) it is possible to employ the same technique as in Sec. IV B. The equations above can be approximated by

$$0 \approx n_\rho n_\nu - G(t,0)\mathcal{I}_{\rho\nu}(t), \quad \rho,\nu = A,B \tag{84}$$

with

$$\mathcal{I}_{\rho\nu}(t) \equiv \Lambda_{\rho\nu}\int_0^t dt'\varphi_{\rho\nu}(t'), \quad \rho = A,B. \tag{85}$$

By integrating Eqs. (81) and (82) a useful relationship can be derived for $\mathcal{I}_{\rho\nu}$, $\rho,\nu = A,B$,

$$\mathcal{I}_{\rho\rho}(t) + \mathcal{I}_{AB}(t) = n_{0,\rho} - n_\rho(t) \approx n_{0,\rho}, \quad \rho = A,B. \tag{86}$$

Using Eqs. (84) and (86) gives

$$(n_A + n_B)^2 \approx G(t)(n_{0,A} + n_{0,B}), \tag{87}$$

$$n_A^2 - n_B^2 \approx G(t)(n_{0,A} - n_{0,B}). \tag{88}$$

Solving the equations above leads to

$$n_\rho \sim \frac{n_\rho(0)}{\sqrt{n_{0,A} + n_{0,B}}}(8\pi Dt)^{-d/4}, \quad \rho = A,B. \tag{89}$$

According to WBGA-I both particles decay with the $d/4$ exponent and amplitudes given above. The WBGA-I predicts the 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 ϵ-expansion analysis of this reaction suggest $d/2$ exponent [18,19]. To see what happens when $O(n^3)$ terms are kept in Eq. (78)–(80) we proceed with WBGA-II calculation.

B. WBGA-II

In the WBGA-II, when all terms are kept in Eqs. (78)–(80), it is useful to rewrite these equations in the vector form

$$\left(\frac{\partial}{\partial t} + 2Dk^2\right)\begin{pmatrix}\Gamma_k^{AA}\\ \Gamma_k^{BB}\\ \Gamma_k^{AB}\end{pmatrix} = -\mathbf{P}(t)\begin{pmatrix}\Gamma_k^{AA}\\ \Gamma_k^{BB}\\ \Gamma_k^{AB}\end{pmatrix} - \begin{pmatrix}\lambda\varphi_{AA}\\ \lambda\varphi_{BB}\\ \delta\varphi_{AB}\end{pmatrix}, \tag{90}$$

where the matrix $\mathbf{P}$ is given by

$$\mathbf{P} = n_A\begin{pmatrix}4\lambda + 2\delta u & 0 & 2\delta\\ 0 & 4\lambda u + 2\delta & 2\delta u\\ \delta u & \delta & (2\lambda + \delta)(1+u)\end{pmatrix} \tag{91}$$

with $u=n_B/n_A$.

Vector equation (90) 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 the *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. (90).

To get the feeling of what follows it is useful to analyze Eqs. (75) and (76) at the mean field level, where fluctuations are neglected by setting $\Phi_{\rho\nu}$ to zero; $\dot{n}_A=-(\lambda n_A^2+\delta n_A n_B)$, and $\dot{n}_B=-(\lambda n_B^2+\delta n_A n_B)$. The mean field equations can be solved approximately for large t (please see Ref. [19] for details) and one obtains

$$n_A\sim\frac{1}{\lambda t},\quad n_B\sim\frac{n_{0,B}}{[n_{0,A}\lambda t]^{\gamma}},\tag{92}$$

provided $\gamma\equiv\delta/\lambda>1$ and $n_{0,A}>n_{0,B}$. For $\delta=\lambda$ ($\gamma=1$) or $n_{0,A}=n_{0,B}$ the 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 (92) and try to solve Eq. (90) with it. The validity of such a mean field ansatz will be checked self-consistently at the end. For large times, and with mean field behavior ($u\to 0$), the matrix $\mathbf{P}$ can be approximated by

$$\mathbf{P}\approx\lambda n_A\mathbf{\Pi},\quad \mathbf{\Pi}=\begin{pmatrix}4&0&2\gamma\\0&2\gamma&0\\0&\gamma&2+\gamma\end{pmatrix}.\tag{93}$$

The fact that $\mathbf{P}$ (in the approximate form) is a constant matrix multiplied by a time dependent function implies that $[\dot{\mathbf{P}}(t),\dot{\mathbf{P}}(t')]=0$ (dot over symbol $\mathbf{P}$ denotes time derivative). This being the case, Eq. (90) can be treated as a scalar equation and a calculation similar to the one in Sec. IV B gives

$$\begin{pmatrix}\varphi_{AA}(t)\\\varphi_{BB}(t)\\\varphi_{AB}(t)\end{pmatrix}=\begin{pmatrix}n_A(t)^2\\n_B(t)^2\\n_A(t)n_B(t)\end{pmatrix}-\int_0^t dt'\,\mathbf{J}(t,t')\begin{pmatrix}\lambda\varphi_{AA}(t')\\\lambda\varphi_{BB}(t')\\\delta\varphi_{AB}(t')\end{pmatrix},\tag{94}$$

where matrix $\mathbf{J}(t,t')$ is given by

$$\mathbf{J}(t,t')=G(t,t')\exp[-\xi(t,t')\mathbf{\Pi}]\tag{95}$$

and

$$\xi(t,t')\equiv\lambda\int_{t'}^t dt''n_A(t'').\tag{96}$$

Please compare Eqs. (44) and (45) and Eqs. (94) and (95). They are very similar, the only difference being in the matrix character of Eqs. (94) and (95). Following the same steps as in Sec. IV B, Eq. (94) can be approximated as

$$\begin{pmatrix}\varphi_{AA}\\\varphi_{BB}\\\varphi_{AB}\end{pmatrix}\approx\begin{pmatrix}n_A^2\\n_B^2\\n_An_B\end{pmatrix}-\mathbf{J}(t,0)\begin{pmatrix}\mathcal{I}_{AA}\\\mathcal{I}_{BB}\\\mathcal{I}_{AB}\end{pmatrix}.\tag{97}$$

Now we proceed to show that, as in the case of Eq. (46), the second term on the right-hand side of Eq. (97) can be neglected.

Matrix $\mathbf{\Pi}$ can be diagonalized as $\mathbf{\Pi}\cdot\mathbf{U}=\mathbf{U}\cdot\mathbf{\Omega}$. The $\mathbf{\Omega}$ is diagonal matrix containing eigenvalues

$$\omega_1=4,\quad \omega_2=2\gamma,\quad \omega_3=2+\gamma\tag{98}$$

and matrix $\mathbf{U}$ contains eigenvectors

$$\mathbf{U}=\begin{pmatrix}1&\dfrac{\gamma}{\gamma-2}&\dfrac{2\gamma}{\gamma-2}\\0&\dfrac{\gamma-2}{\gamma}&0\\0&1&1\end{pmatrix}.\tag{99}$$

Inserting Eq. (92) into Eq. (96), and assuming large t, leads to

$$\xi(t,0)\sim\text{const}+\ln t,\tag{100}$$

and using Eq. (100) in Eq. (95) gives

$$\mathbf{J}(t,0)\sim\text{const}\times t^{-d/2}\mathbf{U}\begin{pmatrix}t^{-4}&0&0\\0&t^{-2\gamma}&0\\0&0&t^{-(2+\gamma)}\end{pmatrix}\mathbf{U}^{-1}.\tag{101}$$

Finally, the second term on the right hand side of Eq. (97) can be calculated explicitly. Inserting Eq. (101) into Eq. (97), and assuming that $\mathcal{I}_{\rho\nu}$ $\rho,\nu=A,B$ are constants (can be checked for self-consistency at the end), results in

$$\varphi_{AA}\approx n_A^2+t^{-d/2}(c_1t^{-\omega_1}+c_2t^{-\omega_2}+c_3t^{-\omega_3}),\tag{102}$$

$$\varphi_{BB}\approx n_B^2+t^{-d/2}c_4t^{-\omega_2},\tag{103}$$

$$\varphi_{AB}\approx n_An_B+t^{-d/2}(c_5t^{-\omega_2}+c_6t^{-\omega_3}).\tag{104}$$

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

To see that the terms originating from $\mathbf{J}(t,0)$ are subleading, one really has to calculate $\mathbf{U}$ explicitly. For example, not knowing that the contribution from ω_1 is absent in Eq. (103), there would be a need to compare $t^{-2\gamma}$ [asymptotics of the mean field n_B^2 term in Eq. (103)] with $t^{-(d/2+4)}$ [coming from $\mathbf{J}(t,0)$ and ω_1 eigenvalue]. One would conclude that γ

$=\delta/\lambda$ cannot be too large if mean field asymptotics is to hold. In reality, there is no such bound on ratio δ/λ since eigenvalue ω_1 does not appear in Eq. (103), but this can only be seen after an explicit calculation.

The main finding so far is that WBGA describes then $ABBA$ and $A+A$ models in the same way. For both models the WBGA-I (WBGA-II) predicts $d/4$ (mean field) density decay exponents. In the following section an attempt will be made to improve the WBGA method in order to obtain the correct value of density decay exponent for the $ABBA$ model.

C. WBGA/Kirkwood approximation applied to $A+A$ and $B+B$ sectors

Unfortunately, WBGA cannot give any reasonable predictions about asymptotic value for particle density ration $u(t)$, as it cannot even get the exponents right. How deep does the weakness of WBGA go? What needs to be changed in equations of motion (78)–(80) in order to get the correct decay exponent? To answer these questions we begin by modifying more and more terms in Eqs. (78)–(80) by using the recipe from Sec. IV C, i.e., the WBGA/Kirkwood scheme. It was already remarked in Sec. II that contributions to H describing different reaction sectors enter additively, and this feature is reflected in equations of motion (78)–(80), which opens a way for such incremental changes.

We begin by modifying terms describing $A+A$ and $B+B$ reactions in equations of motion for AA and BB correlation functions. If one is to follow the procedure described in Sec. IV C, the $O(n^3)$ term in Eq. (78) has to be modified as

$$4\lambda n_A \Gamma_k^{AA} \to 2\lambda \Gamma_k^{AA} \frac{n_A^2 + \Phi_{AA}}{n_A} \tag{105}$$

and likewise for Eq. (79),

$$4\lambda n_B \Gamma_k^{BB} \to 2\lambda \Gamma_k^{BB} \frac{n_B^2 + \Phi_{BB}}{n_B}. \tag{106}$$

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

$$\frac{\partial}{\partial t}\Gamma_k^{AA} = -2Dk^2\Gamma_k^{AA} - \lambda(n_A^2 + \Phi_{AA}) - 2\lambda\Gamma_k^{AA}\frac{n_A^2 + \Phi_{AA}}{n_A} - 2\delta(n_B\Gamma_k^{AA} + n_A\Gamma_k^{AB}), \tag{107}$$

$$\frac{\partial}{\partial t}\Gamma_k^{BB} = -2Dk^2\Gamma_k^{BB} - \lambda(n_B^2 + \Phi_{BB}) - 2\lambda\Gamma_k^{BB}\frac{n_B^2 + \Phi_{BB}}{n_B} - 2\delta(n_A\Gamma_k^{BB} + n_B\Gamma_k^{AB}). \tag{108}$$

Equation (80) stays the same, although Eq. (80) contains a term proportional to λ which should be modified if one follows the principle outlined above. However, at the moment, Eq. (80) will not be changed. The set of equations just described can be conveniently referred to as WBGA/Kirkwood$[AA_\lambda BB_\lambda]$.

To solve the WBGA/Kirkwood$[AA_\lambda BB_\lambda]$ set of equations, it is useful to employ similar notation to the one used in Sec. IV B:

$$\Gamma_k^{\rho\nu} \equiv n_\rho n_\nu \chi_k^{\rho\nu} \tag{109}$$

and

$$\chi_{\rho\nu} \equiv 1 + \frac{1}{V}\sum_{k\neq 0} \chi_k^{\rho\nu} \tag{110}$$

with $\rho,\nu = A,B$. Using Eqs. (109) and (110) in Eqs. (81) and (82) results in

$$\frac{\partial}{\partial t} n_A = -(\lambda n_A^2 \chi_{AA} + \delta n_A n_B \chi_{AB}), \tag{111}$$

$$\frac{\partial}{\partial t} n_B = -(\lambda n_B^2 \chi_{BB} + \delta n_A n_B \chi_{AB}). \tag{112}$$

Implementing the same notation in Eqs. (107), (108), and (80) gives

$$\frac{\partial}{\partial t}\chi_k^{AA} = -2Dk^2\chi_k^{AA} - \lambda\chi_{AA} - 2\delta n_B(1-\chi_{AB})\chi_k^{AA} - 2\delta n_B\chi_k^{AB}, \tag{113}$$

$$\frac{\partial}{\partial t}\chi_k^{BB} = -2Dk^2\chi_k^{BB} - \lambda\chi_{BB} - 2\delta n_A(1-\chi_{AB})\chi_k^{BB} - 2\delta n_A\chi_k^{AB}, \tag{114}$$

$$\frac{\partial}{\partial t}\chi_k^{AB} = -2Dk^2\chi_k^{AB} - \delta\chi_{AB} - [\lambda n_A(2-\chi_{AA}) + \lambda n_B(2-\chi_{BB}) + \delta(n_A+n_B)(1-\chi_{AB})]\chi_k^{AB} - \delta(n_A\chi_k^{AA} + n_B\chi_k^{BB}). \tag{115}$$

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). It can be seen that WBGA/Kirkwood$[AA_\lambda BB_\lambda]$ approach, as expressed in Eqs. (113)–(115), does not describe the $ABBA$ 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). The inspection of individual density decays (not shown here) reveals that the equations above correctly describe the decay of majority species, i.e., $n_A \sim \text{const} \times t^{-d/2}$, but fail to describe the decay of minority species n_B.

To continue this line of incremental changes, in the following more terms will be modified by using WBGA/Kirkwood approach. The dash-dotted line in Fig. 2 shows a solution of equations (not shown here) obtained from modifying $A+A$ and $B+B$ reaction sectors using shortened Kirk-

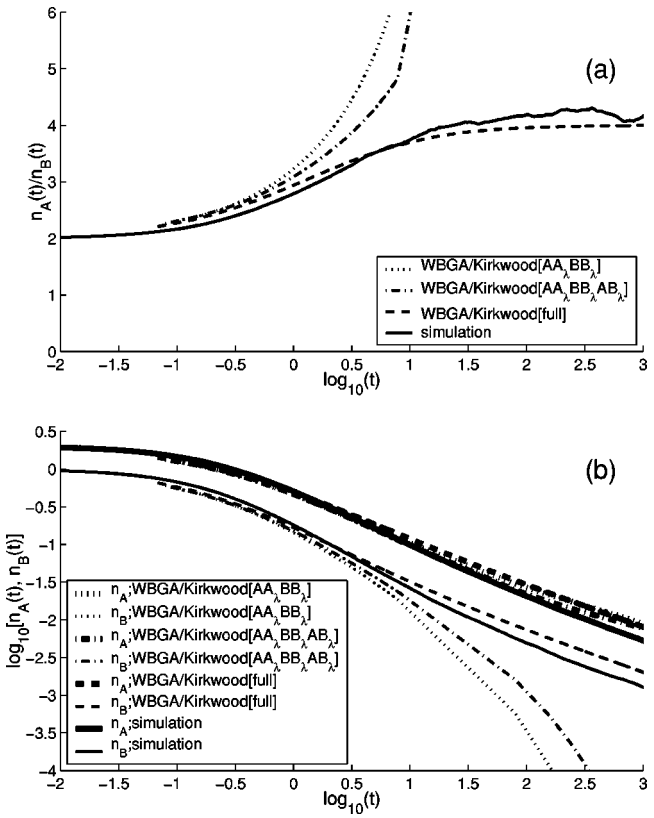

FIG. 2. The numerical solution of Eqs. (111)–(115) for $d=1$ with increasing the amount of WBGA/Kirkwood approximation embedded (dotted, dash-dotted, and dashed lines; please see the text in Sec. VI C for details). The full curve is the result of a Monte Carlo simulation (average of 500 runs). Parameters used are $L=1000$, $n_A(0)=2$, $n_B(0)=1$, $\lambda=1$, and $\delta=2$. Panel (a) shows particle density ratio, panel (b) shows individual densities. In both panels lines are denoted in the same way. Panel (a) shows that only full implementation of the WBGA/Kirkwood approximation scheme qualitatively describes the density ratio. In panel (b) it can be seen that all approximation schemes, apart from WBGA/Kirkwood[full], correctly predict the decay of majority species while failing to describe minority species. WBGA/Kirkwood[full] describes both well. Both panels (a) and (b) show that increasing the amount of WBGA/Kirkwood in equations leads to successively better agreement with the simulation experiment.

wood superposition approximation in Eq. (80) describing time evolution of AB correlation function. These equations will be referred to as WBGA/Kirkwood$[AA_\lambda BB_\lambda AB_\lambda]$. Equations obtained in this way are identical to Eqs. (113)–(115) with the only difference that Eq. (115) changes in a way that terms proportional to λ drop out. In Fig. 2 it can be seen that even in this case the density ratio curve climbs to infinity, which is not the correct behavior, but the overall trend gets better as the dash-dotted curve lies below the dotted one and is pushed towards the simulation curve.

Finally, the equations of motion were studied where even the δ terms (describing the $A+B$ reactions) were modified in equations of motion for all correlation functions. This set of equations will be referred to in the following as WBGA/Kirkwood$[AA_{\lambda,\delta}BB_{\lambda\delta},AB_{\lambda\delta}]$, or even more briefly as WBGA/Kirkwood[full]. Equations obtained in this way are the same as in Eqs. (113)–(115) the only difference being in the fact that all seemingly $O(n)$ terms drop out. Thus in Eqs. (113)–(115) only diffusion term and terms $\lambda\chi_{AA}$, $\lambda\chi_{BB}$, and $\delta\chi_{AB}$ are kept in Eqs. (113), (114), and (115) 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 a dashed line. [It is possible to analytically extract density decay asymptotics for this truncated set of equations which gives $n_A(t)\sim \text{const}\times t^{-d/2}$ and $n_B(t)\sim \text{const}'\times t^{-d/2}$.]

The set of equations where WBGA/Kirkwood superposition approximation has been applied fully agrees with the numerical simulation much better than the ones obtained from partial implementation. This is a strong indication that, at least for the $ABBA$ model, the WBGA/Kirkwood approximation is superior to the WBGA method. For example, in Fig. 2, the trend in all curves improves as the content of the WBGA/Kirkwood approximation is increased. As the goal of the present study is to understand the WBGA method better, the more thorough analysis of the $ABBA$ reaction based on the Kirkwood superposition approximation will be presented in a forthcoming publication.

VII. CONCLUSIONS

The workings of the WBGA were analyzed on reaction-diffusion models with a trivial stationary state but nontrivial dynamics in approaching this state. Admittedly, in doing so, the WBGA approach was taken out of the original sphere of application with focus on highly correlated stationary states. The $A+A$, $A+B$, and $ABBA$ models were used as test cases. The $A+A$ and $A+B$ are excellent test models since they are well understood. In the case of the *ABBA* model, an attempt has been made to calculate particle density ratio $u(t)=n_B(t)/n_A(t)$. Also, some seemingly independent calculation schemes available in the literature were related to each other.

It was shown that the WBGA fails to describe the $A+A$ model, on both WBGA-I and WBGA-II levels. On the other hand, it describes the $A+B$ reaction well, out of pure coincidence so it seems. The failure of the WBGA to describe the $A+A$ model was analyzed in detail at two stages.

(1) It was shown that the WBGA amounts to approximating the three-particle correlation function in a particular way, which corresponds to additive approximation of correlation functions, being already criticized before in the context of fermionic models which allow for single occupancy of lattice sites only.

(2) To cure the deficiency of the WBGA method, a way of approximating three-particle correlation was suggested in the form of Kirkwood inspired the WBGA approximation, referred in the text as the WBGA/Kirkwood approximation. To the best of our knowledge no such approach, nor any other form of the Kirkwood superposition approximation, was ever used to describe bosonic models where multiple occupancy of lattice sites is allowed with extremely local on-site reactions. It was shown that the WBGA/Kirkwood approximation suggested here leads to the correct $d/2$ decay exponent for the $A+A$ reaction.

The equivalence of the WBGA-I and dressed-tree calculation of Ref. [20] was demonstrated, for the case of the $A+A$ reaction. However, it can be easily seen that this equivalence holds for any model where particles annihilate in pairs. Furthermore, it was shown that for the $A+A$ reaction the dressed-tree calculation results in the $d/4$ density decay exponent, and the error in Ref. [20] was corrected. In such a way seemingly contradictory claims of Refs. [20] and [6] were sorted out.

Also, it was shown that the WBGA cannot describe the *ABBA* model, very likely, for the same reasons as the $A+A$ model since these two models fall in the same universality class. In the case of the *ABBA* model the WBGA-II predicts faster vanishing of minority species, which is suggestive of the $(A+B)$-like behavior rather than the behavior of the *ABBA* model as found in Refs. [18,19]. This bias towards $A+B$ type behavior is very hard to get rid of as successively correcting more and more terms in equations of motion for the *ABBA* the model by using the WBGA/Kirkwood approximation results in faster vanishing of minority species. The vanishing of minority species persists until all terms are modified by the WBGA/Kirkwood method. The WBGA simply emphasizes the $A+B$ reaction sector too strongly in the *ABBA* model.

The findings of this work suggest that the formalism employed by Mattis and Glasser in Ref. [6] where a small n_0 expansion is introduced (and applied to study the $A+B$ model) is somewhat questionable. This procedure works on the $A+B$ model, but might not work for other models. It can be shown (by rescaling $a^\dagger n_0 \to a^\dagger$ and $a/n_0 \to a$) that for the type of models studied here, the small n_0 approximation of Ref. [6] amounts to taking away three body terms in the Hamiltonian given in Eq. (5) or (14) (e.g., operators of the type $a^\dagger aa$ and likewise any mixture of a or b operators). Neglect of these terms amounts exactly to the WBGA-I approach, which is criticized here. For these reasons, a small n_0 expansion, which effectively means taking away the three body term in the Hamiltonian, cannot be trusted if used beyond the $A+B$ model.

There is a strong indication from the present analysis that the WBGA/Kirkwood approximation is superior to the WBGA method, at least when applied to the $A+A$ and *ABBA* models. However, it remains to be seen whether the bosonic on-site reaction version considered here, works on the $A+B$ model, which the pure WBGA describes well. Actually, it is likely that it will not work. For example, a similar study (where only single occupancy of lattice sites was allowed and reaction range was assumed short but finite) showed that only the full Kirkwood superposition approximation can describe the $A+B$ reaction [4], while here an equivalent of the shortened Kirkwood superposition approximation was used. Extending the present analysis to the full Kirkwood superposition approximation will amount to keeping all terms in Eq. (58). Extending the WBGA in the direction of the full Kirkwood superposition approximation will be presented in a forthcoming publication.

There is an interesting question about how to implement the decoupling schemes of this work in the case of reaction-diffusion systems of "hard-core" particles, i.e., systems where each site can be at most occupied by one particle. What would be the efficiency of these approximate schemes for these systems? The hard-core constraint may have a dramatic effect on the dynamics in some cases [26]. In one dimension it is possible to reformulate reaction-diffusion systems of hard-core particles in a spin language and then, via a Jordan-Wigner transformation, adopt a fermionic field-theoretical formalism (for detailed instructions on carrying out this procedure see, e.g., Ref. [27]). The present scheme could be applied to the averages involving products of fermionic operators, once the Jordan-Wigner transformation has been made.

To conclude, it would be interesting to have a relatively simple approximation at hand, not far away from the pair approximation, which could be used to extract qualitative asymptotics for an arbitrary reaction-diffusion model, irrespective of which model one studies. Clearly, such a program is ambitious since in reality one is bound to make an 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 benchmark models and any successful approximation should strive to describe these reactions properly. The present study is an attempt in this direction.

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APPENDIX A: TERM MATCHING

Here, the calculation done in Ref. [20] will be repeated to show how to balance terms correctly. Also, the calculation will justify approximations employed in Ref. [6] more rigorously as the method of calculation employs a Laplace transform and the well known Tauberian theorems which relate small s with large t behavior. In this way all the approximations are controlled.

To extract the asymptotic behavior for $n(t)$ from Eq. (42), one assumes that at large times density decays as

$$n(t) \approx \mathcal{A}(\mu + t)^{-\alpha}. \tag{A1}$$

$\mathcal{A}$ and α denote amplitude and exponent of decay to be found. μ is introduced as a regulator for small t so that Laplace transform of $n(t)$ and $n^2(t)$ exist:

$$n(s) = \mathcal{A} e^{s\mu} s^{\alpha - 1} \Gamma(1-\alpha, \mu s), \tag{A2}$$

$$n_2(s) = \mathcal{A}^2 e^{s\mu} s^{2\alpha - 1} \Gamma(1-2\alpha, \mu s), \tag{A3}$$

and please note that $n(s)^2 \neq n_2(s)$. To extract asymptotics one inserts Eqs. (A2) and (A3) and Eq. (41) into Eq. (40), 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

$$g(s)=(8\pi D)^{-d/2}e^{s\eta}\left[\Gamma(1-d/2)s^{d/2-1}+\frac{2\eta^{1-d/2}}{d-2}+O(s)\right] \tag{A4}$$

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

$$g(s)=(8\pi D)^{-1}e^{s\eta}[-\gamma_E-\ln(\eta s)+O(\eta s)], \tag{A5}$$

where γ_E is the 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 below and above $d=2$. For small s and $d<2$ $g(s)\propto s^{d/2-1}$ while for $d>2$ $g(s)=$const. At $d=2$ there is logarithmic dependence on s. The term $e^{s\eta}$ 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 Eq. (41) gives

$$\lambda_{\mathrm{eff}}(s)\sim\frac{(8\pi D)^{d/2}}{\Gamma(1-d/2)}s^{-d/2+1},\quad d<2. \tag{A6}$$

Since the value for α is not known, one has to separate various cases: expansion for $n(s)$ reads

$$n(s)=\mathcal{A}\begin{cases}[\Gamma(1-\alpha)s^{\alpha-1}+O(1)], & \alpha<1\\ \left[\dfrac{\mu^{1-\alpha}}{\alpha-1}+O(s^{\alpha-1})\right], & \alpha>1\end{cases} \tag{A7}$$

and likewise

$$n_2(s)=\mathcal{A}^2\begin{cases}[\Gamma(1-2\alpha)s^{2\alpha-1}+O(1)], & 2\alpha<1\\ \left[\dfrac{\mu^{1-2\alpha}}{2\alpha-1}+O(s^{2\alpha-1})\right], & 2\alpha>1.\end{cases} \tag{A8}$$

Inserting small s expansions (A6)–(A8) into Eq. (40) gives

$$\mathcal{A}[s^{\alpha}\Gamma(1-\alpha)+\mathcal{O}(s)]-n_0 = -\mathcal{A}^2\frac{(8\pi D)^{d/2}}{\Gamma(1-d/2)}[s^{2\alpha-d/2}\Gamma(1-2\alpha)+O(s^{1-d/2})]. \tag{A9}$$

Also, please note that there are two different forms to use for $n(s)$ and $n_2(s)$ in Eqs. (A7) and (A8) and the ones used in (A9) were for $\alpha<1$ and $2\alpha<1$, respectively (same choice was made in Ref. [20]). Once α is found, one has to check these conditions on α for self-consistency. There are two ways to match the terms in Eq. (A9): (a) as in Ref. [20] and (b) in a way related to the work in Ref. [6]. We begin with the first case.

Balancing the s^{α} term on the left hand side of Eq. (A9) with $s^{2\alpha-d/2}$ on the right-hand side gives $\alpha=d/2$ and

$$\mathcal{A}_a=-\frac{1}{\pi}\sin(\pi d)\Gamma(d)\Gamma(1-d/2)^2(8\pi D)^{-d/2}. \tag{A10}$$

Also from $\alpha<1$ and $2\alpha<1$ one has the constraint that $d<1$. However, for $d<1$ the term $\sin(\pi d)$ is positive, which makes the amplitude $\mathcal{A}_a$ negative. Thus all physical conditions cannot be met with this type of matching. In Ref. [20] the condition $d<1$ [coming from the fact that the first row is used in Eq. (A8)] was overlooked (if $d>2$ is allowed, amplitude $\mathcal{A}_a$ is perfectly acceptable).

The $\alpha=d/2$ scenario can still turn out to be true. With this choice of α and the $d<2$ condition coming from Eq. (A6) the second row in Eq. (A8) has to be used. Again, carrying out a 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 the constant n_0 term on the left-hand side of Eq. (A9) with $s^{2\alpha-d/2}$ on the right-hand side. [The remaining terms, e.g., the s^{α} on the left-hand side, can be balanced by considering subleading corrections to $n(s)$.] This way of balancing immediately gives $\alpha=d/4$ and

$$\mathcal{A}_b=\sqrt{n_0}(8\pi D)^{-d/4} \tag{A11}$$

with constraints that $d<2$ [Eq. (A6) was used to get Eq. (A9)].

Matching the constant term n_0 on the left-hand side of Eq. (A9) is rather counterintuitive 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. (40).

Equation (40) comes from Eq. (37). For simplicity we focus on the case $\lambda=\infty$ in Eq. (37). It is clear that at the right-hand side of Eq. (37) the $sn(s)$ term is subleading 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 $\mathcal{A}_b$ obtained previously. Also, by using form (37), one can show that amplitude $\mathcal{A}_b$ as given in Eq. (A11) is valid even for $d>2$. Analysis can be repeated with finite value of λ with the same outcome. It is important to mentioned that procedure outlined above does not work at $d\geqslant 4$ and it has to be modified.

APPENDIX B: DETAILS OF NUMERICAL INTEGRATION

Here, the numerical treatment of Eqs. (33) and (34) is described in more detail. The general procedure for integrating expressions of the type

$$I_i[f]=\int_0^{t_i}dsK(t_i,s)f(s), \tag{B1}$$

where $K(t,s)$ is singular when s approaches t is described in Ref. [28]. The $i=0,1,2,\ldots$ and $t_i=ih$. The following procedure described in Ref. [28], and using $K(t,s)=(t-s+\eta)^{-\alpha}$, results in the quadrature formula:

$$I_i[f]\approx\sum_{j=0}^{i}w_{ij}f(t_j), \tag{B2}$$

where coefficients w_{ij} are given by

$$w_{i0}=\frac{h^{1-\alpha}}{(\alpha-1)(\alpha-2)}[(2-\alpha-i-\eta)(i+\eta)^{1-\alpha} + (i+\eta-1)^{2-\alpha}], \tag{B3}$$

$$w_{ij}=\frac{h^{1-\alpha}}{(\alpha-1)(\alpha-2)}[(i-j+\eta-1)^{2-\alpha}+(i-j+\eta+1)^{2-\alpha} - 2(i-j+\eta)^{2-\alpha}], \tag{B4}$$

$$w_{ii}=\frac{h^{1-\alpha}}{(\alpha-1)(\alpha-2)}[(1+\eta)^{2-\alpha}+\eta^{1-\alpha}(\alpha-\eta-2)]. \tag{B5}$$

The coefficients w_{ij} are chosen from the requirement that Eq. (B2) is exact if $f(t)$ is a piecewise linear function.

The pair of equations in (33)–(34) is discretized as follows. First the differential equation (33) is rewritten in integral form as $n(t)=n_0-\lambda\int_0^t ds\varphi(s)$ and trapezoidal rule is used to evaluate the integral since all functions are well behaved. However, for Eq. (34) the rule (B2) and Eqs. (B3)–(B5) designed for singular kernel is used. Implementation of this philosophy gives

$$n_i=n_0-\lambda h\left[\frac{\varphi_0}{2}+\sum_{j=1}^{i-1}\varphi_j+\frac{\varphi_i}{2}\right], \tag{B6}$$

$$\varphi_i=n_i^2-\lambda\sum_{j=0}^{i-1}w_{ij}\varphi_j-\lambda w_{ii}\varphi_i, \tag{B7}$$

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

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

Here the inverse Laplace transform of $\kappa(s)$ for $d=2$ given in Eq. (66) will be found. Due to the presence of log one has to use the Bramowitz contour to perform integration over s. Also, the function $\kappa(s)$ does not have poles. This means that only contribution to $\kappa(t)$ comes from the branch cut and one obtains

$$\kappa(t)=8\pi D\int_0^\infty\frac{du}{u}e^{-ut}\frac{1}{[\gamma_E+\ln(\eta u)]^2+\pi^2} \tag{C1}$$

In the following we set $\eta=1$ but keep in mind that at the end of the calculation t has to be changed into t/η.

As t grows, due to the presence of $\exp(-ut)$, only smaller and smaller values for u contribute to the integral above, which can be approximated as

$$\kappa\approx(8\pi D)\int_0^c\frac{du}{u}e^{-ut}\frac{1}{(\ln u)^2}, \tag{C2}$$

where c is an arbitrary constant less than 1. It can be shown that the terms omitted or missing the integration range do not influence the leading order behavior for κ. By using partial integration, and change of variables $tu=v$, the expression above becomes

$$\kappa(t)\approx\frac{8\pi D}{\ln t}\int_0^{ct}dv\,e^{-v}\frac{1}{1-\dfrac{\ln v}{\ln t}}. \tag{C3}$$

By sending the upper integration limit to infinity, and expanding the denominator in series over $\ln v/\ln t$, gives the result for $\kappa(t)$ in Eq. (67).

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[16] For example, one way to prepare the system initially is to take a given number of particles and distribute them randomly one by one on the lattice. This way of preparation leads to a Poisson distribution of the particle number at each lattice site. Also, it is clear that preparing the 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.

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[21] In Ref. [20] Eq. (43) of this work is listed as Eq. (54), and appears in a slightly different form. Also, there is a typographical error in the original equation.

[22] The inverse Fourier transform of $\langle a_{k_1} a_{k_2} a_{k_3} \rangle$ is defined as $\langle a_x a_y a_z \rangle = (1/V^{3/2}) \Sigma_{k_1,k_2,k_3} e^{i(k_1 x + k_2 y + k_3 z)} \langle a_{k_1} a_{k_2} a_{k_3} \rangle$.

[23] The Fourier transform of Eq. (55) is calculated by using $\langle a_x a_y \rangle = (/1V) \Sigma_k e^{ik(x-y)} \langle a_k a_{-k} \rangle$. Thus, translational invariance is ensured in the form of $\langle a_x a_y \rangle$. The term $\delta(k_1 + k_2 + k_3)$ appears in Eq. (56) as an artifact of that.

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[25] The density decay amplitude for $A+A$ model is independent of λ and n_0 while the one for $A+B$ model depends only on n_0 (given that systems are observed below critical dimension, naturally).

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