Mean-Field Cluster Approximation Scheme for the Pair-Creation Model with Absorbing Phase Transition

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Abstract

We study the non-equilibrium phase transitions in the one-dimensional pair-creation model \((2A \rightarrow 3A, A \rightarrow 0)\) using the \(n\)-site approximation scheme. We find the phase diagram in the space of the parameters \((\gamma, D)\), where \(\gamma\) is the particle decay probability and \(D\) is the diffusion probability. Through data \((1 \leq n \leq 18)\), we show that in the limit \(n \rightarrow \infty\) the model presents a continuous transition from active state to absorbing state for any value of \(0 \leq D \leq 1\). This result is in contrast with that of Fiore and de Oliveira (Phys. Rev. E 70, 046131, 2004) who found a discontinuous transition at high diffusion regime through conserved order parameter simulations.

Keywords Mean-field cluster · Absorbing phase transition · Pair-creation model

1 Introduction

In recent decades, there has been a great interest of statistical mechanics about one-dimensional systems that exhibit continuous [1–9] and discontinuous [10–16] phase transitions far from equilibrium.

In particular, an argument created by Hinrichsen [17] assures that a single-component model (no longer interactions or additional symmetries) can not present a discontinuous phase transition from an active to an inactive (vacuum) state in one dimension. However, Fiore and de Oliveira [18] through the Monte Carlo simulation reported a tricritical point in high diffusion regime of the pair-creation model (PCM) \((2A \rightarrow 3A, A \rightarrow 0)\).

In order to analyze this apparent divergence, we review the phase diagram of the one-dimension PCM model with diffusion through the \(n\)-site approximation method [19] (mean field cluster approach).

The localization of the tricritical point takes place where the particle density becomes discontinuous (gap) at the transition line (active to absorbing). Therefore, we can study the behavior of the gap \(\Delta \rho_n\) as a function of the cluster approximation \(n = 1, 2, \ldots\) inside the bidimensional parameter space \((\gamma, D)\). Here, \(\gamma\) is the decay probability in the reaction \(A \rightarrow 0\), and \(D\) is the diffusion probability to interchange a monomer \(A\) with near neighbor vacancy.

We will show that in the single mean field approximation \((n = 1)\), the gap \(\Delta \rho_1 = \frac{1}{2}\) between active and absorbing state is constant. Moreover, in the pair site approximation \((n = 2)\), the discontinuity \(\Delta \rho_2 = \frac{D}{4(\gamma + D)}\) is a monotonic function of \(D\). However, in the limit \(n \rightarrow \infty\), we obtain (by extrapolation data) an unphysical tricritical point \((\gamma_t = -0.03865\) and \(D_t = 1.3494)\). This result suggests that the gap \(\Delta \rho_n \rightarrow \infty \rightarrow 0\), and consequently the model, just exhibits a continuous phase transition.

The rest of the paper is organized as follows: in Section 2, we describe the PCM model, whereas in Section 3 the \(n = 1\) and \(n = 2\) mean field approximations are analytically discussed, however the general case \((n \geq 3)\) is just treated numerically; finally, in Section 4 we discuss the results and the limitations of the \(n\)-site scheme.

2 The Model

This model can be seen as an interacting hard core particle model lattice with three processes: spontaneous annihilation (with rate \(\gamma\)), creation particles by two particles (with rate \(s\)), and diffusion of particles (with rate \(D\)). The parameters \(D, s,\) and \(\gamma\) are such that \(D + \gamma + s = 1\).

The configuration of sites in lattice is represented by the vector \(|\beta^n\rangle \equiv |\beta_1\rangle \otimes |\beta_2\rangle \otimes \ldots \otimes |\beta_n\rangle\), in which \(n\) is the
number of sites of lattice. We assume that \( \beta_i \) takes on the value of 1 if the site \( i \) is occupied by a particle and the value of 0 if the site is empty. The evolution rules of the model are as follows.

A site, for example, \( i \) is chosen randomly among the \( n \) sites of the lattice. Suppose \( \beta_i = 1 \), then there are two possible actions: the particle decays with probability \( \gamma \), so the site \( i \) becomes vacant, or it moves to a 2 neighboring site with probability \( D/2 \). Of course, the site \( i \) remains unchanged with probability \( s = 1 - \gamma - D \).

Next, suppose that the site \( i \) is empty, i.e., \( \beta_i = 0 \). The first step is to choose with equal probability (1/2) one of the directions (right or left). Suppose that the right side is chosen, as previously showed, there are two possibilities: occupation of site \( i \) with probability \( s \), provided that \( \beta_{i+1} = \beta_{i+2} = 1 \). If the two sites, which are neighbors of site \( i \), are occupied, then with probability \( s \) a new particle is created, or with probability \( D \) the variables \( \beta_i \) and \( \beta_{i+1} \) are interchanged. A similar procedure is applied in case the neighborhood at the left side of \( i \) is chosen.

### 3 The \( n \)-Site Approximation

Writing the master equation in its continuous-time differential form, we have:
\[
\partial_t |P(\sigma, t)\rangle = \sum_{\beta} w_{(\sigma \rightarrow \beta)} |P(\beta, t)\rangle - w_{(\beta \rightarrow \sigma)} |P(\sigma, t)\rangle,
\]
where \( \sigma, \beta \) represents two distinct lattice configurations. Rewriting (1) in its vector form:
\[
\partial_t |P\rangle = -H |P\rangle,
\]
where \( H \) is a matrix operator responsible for connecting different configurations of the vector space. It is also important to mention that, in general, this operator is not Hermitian, i.e., it has complex eigenvalues. These eigenvalues correspond to the oscillations in the model (imaginary part), while the exponential decay is contained in the real part.

In an orthonormal basis, we have \( \langle \sigma^n | \beta^n \rangle = \delta_{\sigma_1, \beta_1} \delta_{\sigma_2, \beta_2} \cdots \delta_{\sigma_n, \beta_n} \). This suggests that we can write |P\rangle as:
\[
|P\rangle = \sum_{\beta} P(\beta, t) |\beta\rangle.
\]
If we denote the initial probability of the system by
\[
|P_0\rangle = \sum_{\beta} P_0(\beta) |\beta\rangle,
\]
the formal solution of the problem can be written as:
\[
|P\rangle = e^{-Ht} |P_0\rangle.
\]
Due to conservation of probability, we have \( \langle 0 | H = 0 \), where \( \langle 0 | = \sum_{\beta} \langle \beta | \). Thus, any observable can be calculated as follows:
\[
\langle X >_t = \sum_{\beta} X(\beta) P(\beta, t) |\beta\rangle = \langle 0 | X | P\rangle = \langle 0 | e^{-Ht} | P_0\rangle.
\]

However, to compute this amount, it is necessary to diagonalize the evolution operator \( H \). This task is not always viable, since the dimension of this operator \( H \) grows like \( b^n \), where \( b \) is the number of states of a site.

In order to circumvent this difficulty, some numerical procedures are usually adopted, such as Monte Carlo simulations, numerical diagonalization of the operator \( H \) through DMRG scheme, perturbative expansion, and other techniques [17]. Here, we make approximations in the components of the vector |\( P\rangle | \[19 \] and compute its time evolution.

We present now, just as we did in [22], a special scheme to obtain the discrete time evolution of the Master Equation. Since the process is Markovian and the site update rule is independent of \( i \), we can write the component of (1) as:
\[
P_n(\{\sigma^n\}; t + \Delta t) = \sum_{\beta^n} W_{\Delta t}(\{\beta^n\} \rightarrow \{\sigma^n\}) P_n(\{\beta^n\}; t).
\]

Here, \( W_{\Delta t}(\{\beta^n\} \rightarrow \{\sigma^n\}) \) is the conditional probability of the transition from configuration \( \{\beta^n\} \) to configuration \( \{\sigma^n\} \) in the time interval \( \Delta t \). We chose this discrete-time formulation rather than the usual continuous-time approach in order to preserve the interpretation of the parameters \( \gamma, D, \) and \( s \) as probabilities. Using \( W_{\Delta t}(\{\beta^n\} \rightarrow \{\sigma^n\}) = 1 - \sum_{\beta^n \neq \sigma^n} \), we can rewrite (6) in a more convenient form:
\[
\delta P_n(\{\sigma^n\}; t + \Delta t) = \sum_{\beta^n} [W_{\Delta t}(\{\beta^n\} \rightarrow \{\sigma^n\}) P_n(\{\beta^n\}; t)
- W_{\Delta t}(\{\sigma^n\} \rightarrow \{\beta^n\}) P_n(\{\sigma^n\}; t)].
\]

where \( \delta P_n(\{\sigma^n\}; t) = P_n(\{\sigma^n\}; t + \Delta t) - P_n(\{\sigma^n\}; t) \). As usual, the continuous-time formulation is obtained by dividing both sides of (7) by \( \Delta t \), taking the limit \( \Delta t \rightarrow 0 \), and defining \( W_{\Delta t}(\{\beta^n\} \rightarrow \{\sigma^n\})/\Delta t = u(\{\beta^n\} \rightarrow \{\sigma^n\}) \equiv u_{(\beta \rightarrow \sigma)} \) as the transition rate between configurations \( \{\beta^n\} \) and \( \{\sigma^n\} \).

For finite chain sizes, the application of the site update rule \( W_{\Delta t}(\{\beta^n\} \rightarrow \{\sigma^n\}) \) with periodic boundary conditions (i.e., setting \( \sigma_{n+1} = \sigma_1 \) and \( \sigma_0 = \sigma_n \)) allows that the dynamics visit any configurations beginning from an arbitrary initial configuration distinct from the absorbing steady-state \( |\sigma^n\rangle = |0\rangle \) (i.e., the configuration for which \( \sigma_i = 0 \) for \( i = 1, \ldots, n \)). So, the unique steady-state solution of (6) is \( P_n(|\sigma^n\rangle = |0\rangle; t \rightarrow \infty) = 1 \). In the limit of infinitely large chains \( n \rightarrow \infty \), a second stable stationary
solution of (6) appears, the so-called active state for which the average density of particles \( \rho \) is nonzero.

The basic point now is to describe the stochastic dynamics of a \( n \)-site spin configuration only in terms of the joint probability distribution \( P_n(\sigma^n):t \) using translational invariant equations. The condition of translational invariant requires that the update rules for the sites close to the boundaries of the chain are the same as for the inner sites. In order to achieve that, we need to introduce “virtual” [22] sites, say \( i = −1,0 \) if the neighborhood of site \( i = 1 \) is considered. The \( n \)-site approximation is a prescription to write the \( m \)-joint probability distributions \( m > n \) in terms of \( P_n(\sigma^n):t \) only. The basic assumption involved in this approximation scheme is that the states of any two sites are considered as statistically independent variables if their distance is larger than \( n \). For example, we can write \( n + 2 \) jointed distribution \( P_{n+2}(\sigma_−1, \sigma_0, \sigma^{n−2}):t \) as:

\[
Y_{n+2} = \frac{P_n(\sigma_−1, \sigma_0, \sigma^{n−2})}{P_{n−1}(\sigma_0, \sigma^{n−2})} \times \frac{P_n(\sigma_0, \sigma^{n−1})}{P_{n−1}(\sigma^{n−1})} \times P_n(\sigma^n), \tag{8}
\]

where the \( n − 1 \)-site distribution can be easily written in terms of the \( n \)-site distribution (we have omitted the dependence on \( t \) to lighten the notation).

\[
P_{n−1}(\sigma_0, \sigma^{n−2}) = \sum_{\sigma_{−1}=0} P_n(\sigma_−1, \sigma_0, \sigma^{n−2}), \quad \text{and} \quad P_n(\sigma^{n−1}) = \sum_{\sigma_0=0} P_n(\sigma_0, \sigma^{n−2}). \tag{9}
\]

Recalling the update rules PCM model: when the site \( i = 1 \) is empty (i.e., \( \sigma_1 = 0 \)) and its left neighborhood is chosen for the occupation procedure, then it is necessary that its 2 virtual neighbors \( i = −1,0 \) are occupied (i.e., \( \sigma_{−1} = \sigma_0 = 1 \)). In addition, we note that expression (8) is valid for \( n > 2 \) only.

Now, we consider the task of updating the vacant site \( i = 2 \) (i.e., \( \sigma_2 = 0 \)) in a configuration \( |\sigma^n \rangle \) where site \( i = 1 \) is occupied. We need to consider 1 a virtual site \( i = 0 \) and the relevant joint distribution \( Y_{n+1} = P_{n+1}(\sigma_0, \sigma^n) \) is given by:

\[
\langle Y_{n+1} = \frac{P_n(\sigma_0, \sigma^{n−1})}{P_{n−1}(\sigma^{n−1})} \times P_n(\sigma^n), \tag{11}
\]

Next, we present the explicit form of the equations that determine the joint distribution \( P_n(\sigma^n) \) for \( n = 1 \) and \( n = 2 \), referred to as single-site and pair-approximation respectively. In both cases, we derive analytical expressions for the transition point lines and for the jump in the particle density at the transition. For \( n \geq 3 \), we compute the numerical solution of Eq. (7) for the steady-state condition \( \delta P_n(\sigma^n) = 0 \). We solve those \( 2^n \) coupled equations using the Newton-Raphson method with the requisite of an error smaller than \( 10^{-16} \) per equation.

### 3.1 The Single-Site Approximation

The relevant quantity is \( P_1(1) = \rho \), and \( P_1(0) = 1 − \rho \) is given by the normalization condition. Recalling that the only “real” site is \( i = 1 \) and we introduce the convention to write the states of the “virtual” sites (i.e., \( i = −1,0,1,2,3 \)) with an overlying bar. Therefore, we can rewrite Eq. (7) in the form:

\[
\delta P_1(1) = −\gamma P_1(1) + \frac{s}{2} P_3(\bar{1}, \bar{1}, 0) + \frac{s}{2} P_3(0, \bar{1}, \bar{1}). \quad \tag{12}
\]

The diffusion parameter \( D \) does not appear explicitly in this equation because its contribution comes from terms such as \( DP_2(1, 0) \) and \( −DP_2(0, 1) \), which cancel out because of the parity symmetry. Since in this case the sites are statistically independent, we can write \( P_2((1), (1), 0) = P_2^2(1)P_1(0) \) and similarly for the contribution of the right neighborhood of site \( i = 1 \), so that the last equation can be written as:

\[
\delta \rho = −\gamma \rho + s(1−\rho)\rho^2. \tag{13}
\]

The nontrivial solution at stationary state is given by the roots of the equation \( (1−\rho)\rho = \frac{s}{\gamma} \). There is one discontinuous point of particle density \( \Delta \rho \) at the transition between the active and absorbing phases. We find \( \Delta \rho = \frac{1}{2} \) regardless of the values of the control parameters \( \gamma \) and \( D \). Inserting the value \( \rho_1 = \frac{1}{2} \) in the last equation with \( \delta \rho = 0 \) we find the critical value for \( \gamma \).

\[
\gamma_c = \frac{(1−D)}{5}. \tag{14}
\]

### 3.2 The Pair Approximation

In the case \( n = 2 \), (7) can be reduced to only two independent equations using the parity symmetry \( P_2(0, 1; t) = P_2(1, 0; t) \) and their normalization conditions. To illustrate the reasoning that leads to (8) and (11), we will derive the equation for \( P_2(1, 1) \) explicitly. The (7) yields:

\[
\delta P_2(1, 1) = −\gamma P_2(1, 1) − \frac{D}{4} P_3(1, 1, 0) − \frac{D}{4} P_3(\bar{0}, 0, 1, 1)
+ \frac{D}{4} P_3(0, \bar{1}, \bar{1}, 0) + \frac{D}{4} P_3(1, 0, \bar{1}, \bar{1})
+ \frac{s}{4} P_4(\bar{1}, \bar{1}, 0, 1) + \frac{s}{4} P_4(1, 0, \bar{1}, \bar{1})
+ \frac{s}{4} P_3(0, 1, \bar{1}, \bar{1}) + \frac{s}{4} P_3(\bar{1}, 1, 0). \tag{15}
\]
where, as before, we use the convention of writing the virtual site states with an overlying bar. The factor 1/4 appears here because the probability of choosing a given site for update is 1/2 (there are only two real sites) and the probability that the left (or the right) neighborhood of that site is selected to verify the possibility of diffusion (site interchange) or creation is also 1/2.

We begin working with the expressions $P_4(\bar{1}, \bar{1}, 0, 1)$, $P_4(1, 0, \bar{1}, \bar{1})$, $P_3(1, 1, \bar{0})$, and $P_3(1, 0, \bar{1})$. We can rewrite these distribution probabilities as:

$$P_4(\bar{1}, \bar{1}, 0, 1) = \frac{P_2(\bar{1}, \bar{1}) P_2(\bar{1}, 0)}{P_1(\bar{1}) P_1(0)} P_2(0, 1), \quad (16)$$

$$P_4(\bar{1}, \bar{1}, 1, 0) = \frac{P_2(\bar{1}, \bar{1}) P_2(\bar{1}, 1)}{P_1(\bar{1}) P_1(1)} P_2(1, 0), \quad (17)$$

$$P_3(1, 1, \bar{0}) = P_3(0, 1, 1) = P_3(\bar{1}, 1, 0) = 0,$$

$$P_3(0, 1, \bar{1}) = \frac{P_2(0, 1)}{P_1(1)} P_2(1, 1), \quad (18)$$

$$P_3(1, 0, \bar{1}) = P_3(1, 0, \bar{1}) = \frac{P_2(1, 0)}{P_1(0)} P_2(0, 1). \quad (19)$$

At this point, we use the parity symmetry to write $\delta P_2(1, 1)$ given by Eq. (15) in terms of $P_2(1, 1)$ and $P_2(1, 0)$ only. It is still necessary to derive an equation for $\delta P_2(1, 0)$, but this can be done quite straightforwardly using the procedure described above. The final dynamic equations for the pair approximation, posed in terms of usual variables $\phi = P_2(1, 1)$ and $\rho = P_1(1) = P_2(1, 1) + P_2(1, 0) = \phi + P_2(1, 0)$, are:

$$2\gamma \rho = -\gamma \rho + s(\rho - \phi) \frac{\phi}{\rho}, \quad (20)$$

$$2\gamma \phi = -2\gamma \phi + s \frac{\phi}{\rho} \rho - \phi (1 + \frac{\rho - \phi}{1 - \rho}) - D(\rho - \phi^2) \frac{\rho - \phi}{\rho (1 - \rho)}. \quad (21)$$

Different from single-site approximation, here the diffusion parameter $D$ introduces a nontrivial contribution to the component of the master equation. The stationary regime is now obtained from the solution of (20) and (21) which determine the point of the phase transition. In fact, the reduced variable $\phi = \phi/\rho$ is given by the same equation discussed in the single-site approximation and so $\phi = \frac{1}{2}$ at the transition line. This implies that the equation of the transition line $\gamma_c(D)$ is also identical to that obtained in the single-site approximation. However, the size of the discontinuity $\Delta \rho$ at the transition differs in two approximation schemes. Imposing the steady-state condition in the last equation yields:

$$\Delta \rho_2 = \frac{1}{4} \frac{D}{(\gamma_c + D)}, \quad (22)$$

where $\gamma_c$ is given by (14). We note that the equations for the transition line $\gamma_c(D)$ coincide only in the cases of a single-site and pair approximations. The gap density $\Delta \rho$ vanishes from the pair approximation when $D = 0$.

### 3.3 The General $n$-Site Approximation

When $n \geq 3$, we have to resort to a numerical implementation of (7). In particular, the configurations $|\sigma^n>$ (i.e., the
arguments of the joint distribution $P_n$ are represented by $n$ bit integers, which allow an easy implementation of the boundary sites update rules by the Fortran 95 bit intrinsic functions. We chose an initial configuration such that $P(\sigma^n = 1 > 0) \approx 1$ in order for the Newton-Raphson method to find the steady-state solution of Eq. (7).

In the absence of diffusion ($D = 0$), the single site approximation ($n = 1$) predicts a discontinuous phase transition between the absorbing and active phases, while for $n \geq 2$ the transition is always continuous (see Fig. 1). Moreover, the extrapolation data for $\gamma_c^\infty$ converges (as from $n \geq 13$) to 0.12011 ± 0.00001 (see Fig. 2), whereas the Monte Carlo simulation predicts $\gamma_c^{MC}(D = 0) = 0.11971$. However, when $D \neq 0$, we observed that the tricritical point is located in the non-physical regimes $\gamma_t = -0.03865$ and $D_t = 1.3494$, suggesting that the model does not exhibit a tricritical point.

In general, we obtain for single-site and pair approximations the exactly expression for $\gamma_c(n = 1, D)$ and $\Delta_c(n = 2, D)$, respectively.

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References

1. H.K. Janssen, Z. Phys. B 42, 151 (1981)
2. E. Domany, W. Kinzel, Phys. Rev. Letters 53, 311 (1984)
3. P. Grassberger, Z. Phys. B 47, 365 (1982)
4. J.L. Cardy, R.L. Sugar, J. Phys. A 13, L423 (1980)
5. P. Grassberger, J. Phys. A 22, 3673 (1989)
6. R.C. Brower, M.A. Furman, M. Moshe, Phys. Letters 76B, 213 (1978)
7. P. Grassberger, K. Sundemeyer, Vol. 77B68 (1978)
8. H. Takayasu, A.Y.U. Tretyakov, Phys. Rev. Letters 68, 3060 (1992)
9. I. Jensen, Phys. Rev. E 47, 1 (1993)
10. N. Menyhárd, G. Odor, J. Phys. A 31, 6771 (1998)
11. M.R. Evans, Y. Kafri, H.M. Koduvely, D. Mukamel, Phys. Rev. E 58, 2764 (1998)
12. F. Wijland, K. Oerding, H.J. Hilhorst, Physica A, Physica A 251, 179 (1998)
13. C. Codreche, J.M. Luck, M.R. Evans, S. Sandow, D. Mukamel, E.R. Speer, J. Phys. A. Math. Gen. 28, 2039 (1995)
14. D.S. Maia, R. Dickman, J. Cond. Matter 19, 065143 (2007)
15. G. Odor, N. Boccara, G. Szabó, Phys. Rev. E 48, 3168 (1993)
16. R.J. Glauber, J. Math. Phys 4, 4191 (1963)
17. H. Hinrichsen, arXiv:cond-mat/0006212 (2000)
18. C.E. Fiore, M.J. de OLiveira, Phys. Rev. E 70, 046131 (2004)
19. D. ben-Avraham, J. Kühler, Phys. Rev. A 45, 8358 (1992)
20. N.G. Van Kampen, Stochastic Process in Physics and Chemistry, Amsterdam-North-Holland (1981)
21. F.C. Alcaraz, M. Droz, M. Henkel, V. Rittenberg, Annals Phys. 230, 250 (1994)
22. A.A. Ferreira, J.F. Fontanari, J. Phys. A,: Math. Theor. 42, 085004 (2009)

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